Optimal power and resource-intensive process design under uncertainty

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Abstract: Approach to the solution of a problem of optimal power and resource-intensive process design under uncertainty is proposed. The problem has a form of two-stage optimization problem with separate chance constraints. The approach based on the problem’s functions approximations allows us to avoid calculation of multiple integrals. This allows us to reduce the problem of stochastic nonlinear programming to the usual problem of nonlinear programming.

Introduction

It is known that the design of optimal power and resource-intensive processes occurs with partial incompleteness and inaccuracy of information, on the basis of which the designer receives a decision. For modern energy- and resource-intensive industries, uncertainties are caused by inaccuracies in the operation of the control system at associated processes, catalyst deactivation, changes in the heat exchange and mass-exchange characteristics of the apparatus. At the same time, we do not have the opportunity to regulate such impacts that affect the quality of the designed process work. We can only record such changes. Obviously, the refusal to take into account in the formulation of the optimal process design problem of the existing uncertainty can lead to a violation of the requirements for the process functioning or significantly increase the cost of the designed process.

A few approaches to account for uncertainty in optimization have been proposed [1], such as stochastic programming, robust optimization, approximate dynamic programming, and chance-constrained optimization, which is the focus of this article. In this case, the requirements for the work of production can be formulated in the form of hard or chance constraints, depending on the completeness of information on the parameters characterizing the uncertainty, and the preferences of the designer. Hard constraints imply the satisfaction of project requirements at any time during the specified period of production operation. Chance constraints can be represented as separate or joint probability constraints. This form allows us to meet project requirements with a given level of probability. Usually such a probability level is set very high [2].

Accounting for the uncertainty in the criterion of the stochastic programming problem is often presented in the form of a mathematical expectation of some function. Usually this is a function of assessing the process efficiency over the period of process operation. This period is set by the designer. A criterion of pessimism is also used, where the objective function is the worst value of the process
efficiency function over the period. Often the forecast of such a criterion is mitigated by the objective function in the form of the probability boundary of the process efficiency function. The change in the operating conditions of the process is represented by the values of uncertain parameters.

It is obvious that the use of probability constraints and a criterion in the form of expectation or in the form of a probability boundary presuppose the existence of information about the law of distribution of uncertain parameters. In addition to these features, the formalization of optimal process design problems should take into account information from different stages of process life. The most common is the accounting of design and operation stages. Problem in the two-stage optimization problem (TSOP) form is used in the case of obtaining exact values of uncertain parameters from the operation stage and there is the possibility of changing the process operating mode during its operation. This impose an automated control system for the projected process. In other case the one-stage optimization problem (OSOP) form is used. Further we will assume that the uncertain parameters have a normal distribution, are uncorrelated, and their distribution functions are known. As the considered problem of designing an optimal process, we will consider TSOP with separate probability constraints (TSOPSPC).

Formulation of optimization problems with separate chance constraints

Using the objective function in the expected value form we can formulate TSOPSPC in the form:

$$\min_{d,\theta} E[f(d, z(\theta), \theta)]$$

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

where functions $g_j$ are the left part of the inequality constraints, corresponding to design specifications, $\theta$ – $n_\theta$-vector of uncertain parameters, $d$ – $n_d$-vector of design variables, $z(\theta)$ – $n_z$-vector of control variables, $f(d, z(\theta), \theta)$ – function of assessing the process efficiency, $\alpha_j$ – a probability level. Functions $z(\theta)$ characterize the change in the process operating mode, depending on the operating conditions changing. We assume the functions $f$ and $g_j$, $j = 1,\ldots, m$, are continuously differentiable. Value ranges of the parameters $\theta$ form a uncertainty region $T = \{\theta: \theta^i \leq \theta \leq \theta^i, i = 1,\ldots, n_\theta\}$.

To indicate in the problem formulation the possibility of adjusting the operating mode of the project under the changing operating conditions we use functional dependence of the control variables $z$ on the uncertain parameters $\theta$. The indication of this dependence is a characteristic feature of the TSOP. In case of using of the probability boundary of the function $f(d, z(\theta), \theta)$ over the selected process operation period we can formulate the problem in the following form:

$$\min_{d,\theta} q$$

$$\text{Pr}\{g_j(d, z(\theta), \theta) \leq 0\} \geq \alpha_j, \ j = 1,\ldots, m, \quad (4)$$

$$\text{Pr}\{f(d, z(\theta), \theta) \leq q\} \geq \alpha_0. \quad (5)$$

In the problem (1)-(2) the objective function has the form $E_{\theta}[f(d, z(\theta), \theta)] = \int_T f(d, z(\theta), \theta) \rho(\theta) d\theta$, and functions of the constraints left parts have forms:

$$\text{Pr}\{g_j(d, z(\theta), \theta) \leq 0\} = \int_{\Omega_j} \rho(\theta) d\theta, \ \Omega_j = \{\theta: g_j(d, z(\theta), \theta) \leq 0, \theta \in T\}.$$
Here $\rho(\theta)$ – is the probability density function. Because the parameters $\theta$ are uncorrelated, the function has the form $\rho(\theta) = \rho(\theta_1)\rho(\theta_2)...\rho(\theta_{n\theta})$, where $\rho(\theta_i)$ – is the probability density function of the separate uncertain parameter $\theta_i$, $i = 1,...,n\theta$.

In the problem (3)-(5) the left part of the constraint (5) should be calculated as:

$$\Pr\{f(d,z(\theta),\theta) \leq q\} = \int_{\Omega_q} \rho(\theta)d\theta, \Omega_q = \{\theta: f(d,z(\theta),\theta) \leq q, \theta \in T\}.$$  

**Main issues**

The optimization problem with chance constraints was introduced in a work by Charnes et al. [3]. There are many challenging aspects of solving chance constraints optimization problems. The main issues in solving chance constraints optimization problems are the computation of multiple integrals for the calculation of the probabilities of constraint satisfaction (which is very computationally intensive) and the often nonconvex nature of the feasible region of chance-constrained optimization problems. To avoid these difficulties, existing approaches for solving chance constraints optimization problems rely on solving an approximation problem. Generally, three groups of approximation methods are used to approximate chance constraints optimization problems: improvement of the Gauss quadrature, sampling-based approaches, and analytical approximation approaches. The second group of methods contains two categories of techniques: scenario approximation and sample-average approximation. Research contributions in the development of scenario approximation methods have been made by Shapiro and co-workers [4] among others. However, the scenario approximation itself is random, and its solution might not satisfy the chance constraints [5]. Sample-average approximation methods use an empirical distribution associated with random samples to replace the actual distribution and to evaluate the chance constraints. The third group of methods is divided into three categories of techniques: robust optimization, well-known probability inequalities, and the transformation of chance constraints into deterministic constraints. The approaches for obtaining robust solutions to optimization problems have been studied by Floudas and co-workers in a article [6] in which both continuous (general, bounded, uniform, normal) and discrete (general, binomial, Poisson) uncertainty distributions were considered and the framework was applied to operational planning problems. Approaches based on the transformation of chance constraints into deterministic constraints allows the calculation of multiple integrals to be avoided. However, except for a few specific probability distributions (e.g., normal distribution), it is difficult to formulate an equivalent deterministic constraint for a chance constraint. Li et al. [7] proposed a back-mapping method for solving a steady-state OSOP based on the use of the monotonic relationship between the constrained output and one of input uncertain parameters. Geletu et al. [8] proposed a new approach for solving a nonconvex OSOP with non-Gaussian distributed uncertainties. However, their approach still requires the calculation of multiple integrals. Significantly less attention has been paid to the formulation and solution of the TSOP for chemical processes with chance constraints. Ostrovsky et al. [9, 10] formulated the two-stage optimization problem with chance constraints and developed a method for solving this type of problem based on the transformation of chance constraints into deterministic constraints and the partition of the uncertainty region for the cases when the uncertain parameters have a normal distribution. However, proposed approach formulate the problem whose dimension grows exponentially from iteration to iteration. In this article, we develop a new approximate method for solving optimization problems with separate chance constraints for the case when the uncertain parameters are independent random variables. Our method is based on the transformation of chance constraints into deterministic form.
Main approximations

Consider the approximation for the functions $z_r(\theta), \ r=1,...,n_z$. We will use linear in the parameters $\theta$ functions $\bar{z}^q = b_0^q + \sum_{i=1}^{n_\theta} b_i^q \theta^q_i$, where $\theta^q_i - i$-th coordinate of some point $\theta^q \in T$.

Use function $\tilde{f}(d,\bar{z}^q,\theta,\theta^q)$ to approximate functions $f(d,z(\theta),\theta)$, where $\tilde{f}$ is the linear part of the expansion of the function $f$ in a Taylor series at the point $\theta^q$:

$$\tilde{f}(d,\bar{z}^q,\theta,\theta^q) = f(d,\bar{z}^q,\theta^q) + \sum_{i=1}^{n_\theta} \left( \frac{\partial f}{\partial \theta_i} (d,\bar{z}^q,\theta^q) \right) (\theta_i - \theta^q_i).$$ (6)

Let partition uncertainty region $T$ into subregions $T_q = \{ \theta : \theta^q_i \leq \theta_i \leq \theta^q_i + 1, i=1,...,n_\theta \}, \ q = 1,...,Q^{(k)}$, at the $k$-th iteration to improve proposed approximations

$$T = \bigcup_{q=1}^{Q^{(k)}} T_q, \ T_q \cap T_{q_2} = \emptyset, \ q_1,q_2 = 1,...,Q^{(k)}, \ q_1 \neq q_2.$$ (7)

The function $z(\theta)$ approximation has the form $\bar{z} = \{ \bar{z}^q = \{ \bar{z}^q_1,...,\bar{z}^q_{n_z} \}, q = 1,...,Q^{(k)} \}$, and the (1)-(2) problem criteria approximation has the form [2]:

$$E_{\theta^q}[f(d,\bar{z}(\theta),\theta)] = \sum_{q=1}^{Q^{(k)}} \left( \sigma_f(d,\bar{z}^q,\theta^q) + \sum_{i=1}^{n_\theta} \frac{\partial f}{\partial \theta_i} (d,\bar{z}^q,\theta^q) (E[\theta_i;T^{(k)}_q] - a_q \theta^q_i) \right),$$

$$E[\theta_i;T^{(k)}_q] = \left[ \prod_{q=1}^{Q^{(k)}} \Phi(\tilde{\theta}_i^{(k)};a_q) - \Phi(\tilde{\theta}_i^{(k)};a_q) \right] \cdot I_{a_q} \cdot \left[ \prod_{q=1}^{Q^{(k)}} \Phi(\tilde{\theta}_i^{(k)};a_q) - \Phi(\tilde{\theta}_i^{(k)};a_q) \right], \ a_q = \left[ \prod_{q=1}^{Q^{(k)}} \Phi(\tilde{\theta}_i^{(k)};a_q) - \Phi(\tilde{\theta}_i^{(k)};a_q) \right] \cdot I_{a_q} = \int_{\theta_i}^{\theta_i + 1} \theta_i \rho(\theta)d\theta,$$

where $\Phi(\tilde{\theta})$ is the standard distribution function, $E[\theta_i]$ is a mean value and $(\sigma_i)^2$ is the variance of parameter $\theta_i$, $\tilde{\theta}_i^{(k)} = (\theta_i^{(k)} - E[\theta_i]) / \sigma_i$.

Using the $\bar{z}^q$ form, one can get $E_{\theta^q}[f(d,\bar{z}(\theta),\theta)] = \sum_{q=1}^{Q^{(k)}} E_{\theta^q}[f(d,b^q,\theta)]$, where

$$E_{\theta^q}[f(d,b^q,\theta)] = \sigma_f(d,b^q,\theta^q) + \sum_{i=1}^{n_\theta} \frac{\partial f}{\partial \theta_i} (d,b^q,\theta^q) (E[\theta_i;T^{(k)}_q] - a_q \theta^q_i), \ q = 1,...,Q^{(k)},$$ (8)

and $b^q = \{ b^q_0, b^q_1,...,b^q_{n_\theta} \}$, $b^q_i = \{ b_i^{q+1}, b_i^{q+2},...,b_i^{n_\theta} \}, \ q = 1,...,Q^{(k)}$.

Chance constraints transformation

Let transform chance constraints into deterministic ones. Firstly, we consider the method of transforming constraints (2), which we extend below to constraints (5). We use the method for the linear in parameters $\theta$ function $g(x,\theta) = \theta_1 h_1(x) + ... + \theta_{n_\theta} h_{n_\theta}(x) - c$, $h_i(x), \ i = 1,...,n_\theta$, - arbitrary functions, $c$ - random parameter with an expected value $E[c]$ and a variance $(\sigma_c)^2$. In [11] it is shown that probability constraint $Pr\{g(x,\theta) \leq 0 \} \geq \alpha$ may be transformed into form

$$\sum_{i=1}^{n_\theta} E[\theta_i] h_i(x) + \Phi^{-1}(\alpha)[\sum_{i=1}^{n_\theta} (\sigma_i)^2 h_i(x)^2 + (\sigma_c)^2]^{1/2} \leq E[c].$$ (9)
For case of OSOP we proposed approximation of the functions \( g_j \), by the \( \tilde{g}_j(d, \tilde{z}^q, \theta, \Theta^q) \) - linear part of the their Taylor series expansion at the points \( \theta^{(i)} \in T, \ j = 1, \ldots, m \) [12]. One have the form similar to the (6). We propose in [12] new form of the constraint (9) using following form of the functions \( c_j = \sum_{i=1}^{a_n}(\theta^{(i)} \cdot \tilde{g}_j(d, z, \theta^{(i)}) / \partial \theta_i - g_j(d, z, \theta^{(i)})) \) and \( h_j(d, z) = \tilde{g}_j(d, z, \theta^{(i)}) / \partial \theta_i \),

\[
[c_j - \sum_{i=1}^{a_n}E[\theta_i] \tilde{g}_j(d, z, \theta^{(i)}) / \partial \theta_i] / \sum_{i=1}^{a_n}(\sigma_i \cdot \tilde{g}_j(d, z, \theta^{(i)}) / \partial \theta_i)^2)^{1/2} \geq \Phi^{-1}(\alpha_j) \].

(10)

Let us extend this approach to the TSOPSPC. Since (7) is hold, we can write

\[
\Pr\{g_j(d, z(\theta), \theta) \leq 0\} = \int_{\Omega_{\nu,j}} \rho(\theta)d\theta + \ldots + \int_{\Omega_{\nu,j}^{(i-1)}} \rho(\theta)d\theta, \ j = 1, \ldots, m,
\]

(11)

\[
\Omega_{\nu,j} = \{\theta: g_j(d, z(\theta), \theta) \leq 0, \theta \in T_j\}, \ q = 1, \ldots, Q^x, \ j = 1, \ldots, m.
\]

(12)

Let us use the same points \( \theta^q \) for the expansion of functions \( g_j(d, z(\theta), \theta) \) and \( f(d, z(\theta), \theta) \) taking account of the \( z(\theta) \) approximation in form of the function \( \tilde{z}^q \).

Taking into account the linear approximation of the functions \( g_j(d, z(\theta), \theta) \) one can write the form of the \( q \)-th summand in the (11)

\[
\int_{\Omega_{\nu}} \rho(\theta)d\theta = a_q \Phi \left( c_{q,j} - \sum_{i=1}^{a_n}[E_\theta[\theta_i] \tilde{g}_j(d, b^q, \Theta^q) / \partial \theta_i] \right) \left[ \sum_{i=1}^{a_n}[\sigma_i \cdot \tilde{g}_j(d, b^q, \Theta^q) / \partial \theta_i]^2 \right]^{1/2} \Phi^{-1}(\alpha_j).
\]

(13)

Due to the assumed independence of the uncertain parameters, we get

\[
E_\theta[\theta_i] = \int_{T_j} \theta_i \rho(\theta)d\theta, \quad \sigma_i^q = E_\theta[\theta_i^2] - \left( E_\theta[\theta_i] \right)^2.
\]

(14)

It is clear the expressions (13) do not depend on the search variables of the problem (1)-(2) and can be calculated before problem (1)-(2) solving. Taking into account (10) and (13), (14) we can get deterministic approximation of the constraint (2) in the form

\[
\sum_{q=1}^{Q^q} \left( a_q \left( c_{q,j} - \sum_{i=1}^{a_n}[E_\theta[\theta_i] \tilde{g}_j(d, b^q, \Theta^q) / \partial \theta_i] \right) \left[ \sum_{i=1}^{a_n}[\sigma_i \cdot \tilde{g}_j(d, b^q, \Theta^q) / \partial \theta_i]^2 \right]^{1/2} \right) \geq \Phi^{-1}(\alpha_j),
\]

(15)

where \( c_{q,j} = \sum_{i=1}^{a_n}(\theta^{(i)} \cdot \tilde{g}_j(d, b^q, \Theta^q) / \partial \theta_i) - g_j(d, b^q, \Theta^q), \ j = 1, \ldots, m \).

Using (8), (15) and expressions for the \( \tilde{z}_j^q \) we can write TSOPSPC in the form of the deterministic nonlinear programming
\[ F^{(k)} = \min_{d,b^q} \sum_{q=1}^{Q^{(k)}} E_{q^*}[f(d,b^q,\theta)] \]  

\[ \sum_{q=1}^{Q^{(k)}} q_{q^*} \left( s_q - \sum_{i=1}^{n_q} \left[ E_{q}[\theta_q] \cdot \hat{c}_f(d,b^q,\theta^*) \right] \right) \left[ \sum_{i=1}^{n_q} \left( \sigma_{i,q} \cdot \hat{c}_f(d,b^q,\theta^*) \right) \right]^{0.5} \geq \Phi^{-1}(\alpha_j), \quad j = 1,\ldots,m. \] 

We can solve problem (16) using a nonlinear programming method (for example, the sequential quadratic programming (SQP) method [13]).

It is clear the way of transforming constraints (2) is easily extended to the transomation (5) using linear approximation (6) for the function \( f(d,z(\theta),\theta) \). The constraint (5) get the form

\[ \sum_{q=1}^{Q^{(k)}} \left( s_q - \sum_{i=1}^{n_q} \left[ E_{q}[\theta_q] \cdot \hat{c}_f(d,b^q,\theta^*) \right] \right) \left[ \sum_{i=1}^{n_q} \left( \sigma_{i,q} \cdot \hat{c}_f(d,b^q,\theta^*) \right) \right]^{0.5} \geq \Phi^{-1}(\alpha_q), \]

where \( s_q = \sum_{i=1}^{n_q} [\theta^*_i \cdot \hat{c}_f(d,b^q,\theta^*)] \)- \( f(d,b^q,\theta^*) \).

**Partition of the uncertain region**

Let consider the partition rule to improve the approximation. Let us partition uncertain region \( T \) into subregions \( T_q, \quad q = 1,\ldots,Q^{(k)} \). We should partition the subregion \( T_q \) with the worst quality of the approximation of the function \( f(d,z(\theta),\theta) \) by the function \( \hat{f}(d,z^*,\theta,\theta^*) \) and the total error of the approximation of the functions \( g_j \) by the functions \( \bar{g}_j \) will be the worst. Let \( d^{(k)},b^{(k)q} \) is the problem (1)-(2) solution. To find the \( q^* \) we will use the argument of the following problem solution:

\[ \max_{d,b,q} \max_q \left[ (f(d,b^q,\theta) - f(d,b^{(k)q},\theta,\theta^*))^2 + \sum_{j=1}^{m} (g(d,b^{(k)q},\theta) - \bar{g}(d,b^{(k)q},\theta,\theta^*))^2 \right]. \]

Note that the proposed approach improve the approximation of function \( f(d,b,\theta) \) and functions \( g_j(d,b,\theta), \quad j = 1,\ldots,m \), gradually, from iteration to iteration, which reduces computational costs at the first iterations.

The proposed approach was tested on a model example of the optimal design problem of a system consisting of a reactor and a heat exchanger [14]. Comparison of the obtained results with the results of known approaches [2, 9, 14] showed the effectiveness of the proposed approach, while achieving a significant reduction in time to solve the problem.

**Conclusions**

We proposed an approach for solving problem the design of optimal power and resource-intensive processes under uncertainty. The problem is formulated in the form of the optimization problems with separate chance constraints for cases when the uncertain parameters are independent random variables with arbitrary probability distributions. It is based on the three following steps: approximate transformation of the chance constraints into deterministic ones; approximate calculation of the expected value of the objective function with the help of the piecewise-linear approximation of the
objective function; approximate representation of the control variables $z(\theta)$ as piecewise-constant functions.

To improve these approximations, partition of the uncertainty region into subregions is performed at each iteration. The proposed method excludes multiple integration. In addition, we proposed the approach for solving the TSOPSPC. Li at al. [7] considered only the method for OSOP. The computational experiment showed that the proposed approach decreases significantly the computational time of solving the TSOPSPC for the design problems of the chain of continuous stirred tank reactor and heat exchanger.

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