CHANCE CONSTRAINED BATCH DISTILLATION PROCESS OPTIMIZATION UNDER UNCERTAINTY*

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Abstract

Uncertainties may have a large impact on equipment decisions, plant operability, and economic analysis. Thus the consideration of uncertainties in optimization approaches is necessary for robust process design and operation. As a part of it, efficient chance constrained programming has become an important field of research in process systems engineering. In this work, a new approach is proposed for chance constrained programming of large scale nonlinear dynamic systems, in which some dependent variables at certain time points are to be constrained with a predefined probability. This new approach is an extension and a modification of the existing method for nonlinear chance constrained process optimization, which has been utilized for steady state processes. The main idea of this method is the employment of the monotone relation between output constraints and uncertain variables, so that the probabilities and their gradients can be achieved by numerical integration of the probability density function of the multivariate uncertain variables by collocation on finite elements. The new approach involves new efficient algorithms for realizing the required reverse projection and hence the probability and gradient computation with an optimal number of collocation points so that the original idea is now applicable for dynamic optimization problems with larger scale. This approach is applied for optimization problems of batch distillation with A detailed dynamic process model

Keywords

batch distillation, uncertainty, chance constraints, probabilistic programming.

Introduction

Most current approaches for process operations are based on deterministic optimization, where uncertainties of several parameters are not taken into consideration. Thus systematic methods are required for integrating the available stochastic information of uncertain parameters into process operation decisions.

A process may have internal uncertainties such as inaccurate model parameters or external uncertainties such as unknown future feedstock. However, changing market conditions lead to frequent disturbances from the amount and quality of both feedstock and product. These disturbances are often multivariate and correlated stochastic sequences, which will have influences like a chain-effect, to each unit operation of the production line. The characteristics of the stochastic processes, such as mean, covariance or probability distribution function (PDF), may be known from long term operation data.

To solve an optimization problem under uncertainty, some special treatments of the objective function, the equality and inequality constraints have to be considered in order to relax the stochastic problem to an equivalent NLP problem, so that it can be solved by the existing optimization routines. While the objective function is usually described by the expected value, inequality constraints can be relaxed to chance constraints as one of the main approaches.

In this research we concentrate on the assumption of multivariate normal distributions of the uncertain variables. Thus we finally deal only with NLP problems. For the optimization itself, we use the sequential approach with a

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standard NLP solver. However, the main challenge of this research work lies in the computation of probabilities and their gradients in the simulation layer, especially when the relation between the uncertain and constrained variables is *nonlinear*. Due to the importance of this matter, the expression *nonlinear* is used for describing the relation between those two variables in this context.

The application of the developed stochastic methodology to handle uncertainties of the operation problem under chance constraints to the batch distillation process is the main focus of this contribution.

Method for nonlinear chance constrained programming

In nonlinear systems, the type of the PDF of the uncertain input is not the same as the one of the constrained output. Unlike linear systems, a multivariate normal distribution of the input never causes a multivariate normal distribution of the output. The PDF of the output is mostly not even known. Thus a transformation performed for linear systems is not possible. The chance constraints can be either computed through efficient sampling techniques (Diwekar et al., 1997) or numerical integration techniques (Bernardo et al., 1999). The latter one has been accomplished (Wendt et al. 2002) in the case of a monotone relation between the constrained output and at least one uncertain input. This method is applicable to all stochastic optimization problems with *single* chance constraints.

In this method, an equivalent representation of the probability is derived by mapping the feasible region to a region of the random inputs. Consider the confined feasible region that will be formed by the nonlinear projection from the region of the uncertain variables at some given u. For a practical engineering problem, it is realistic that one can find a monotone relation between an output variable $y_i \in Y_i$ and one of the uncertain input variables $\xi_S \in \Xi_S$, where Ξ_S is a subspace of Ξ. Denoting this monotone relation as $y_i = F(\xi_S)$, the mapping between y_i and ξ_S can be schematically depicted in Fig. 1.

The right and left circle in Fig. 1 represent the whole region of Y_i and Ξ_S respectively. The points are some realizations of the variables based on their distribution functions. A point in Ξ_S leads to a point in Y_i through the projection $y_i = F(\xi_S)$. Due to the monotony, a point y_i can lead to a unique ξ_S through the reverse projection $\xi_S = F^{-1}(y_i)$. The shaded area in the right circle is the output feasible region Y_i' such that

$$P\{y_i \le y_i^{SP}\} \ge \alpha \qquad (1)$$

is satisfied, while the shaded area Ξ_S' in the left circle is

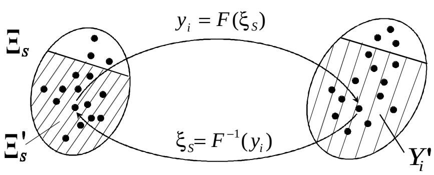

Fig. 1: Mapping between an uncertain input variable and an output variable.

the region, with the bound ξ_S^L, of the random variable corresponding to Y_i'. It can be easily seen that if $y_i \uparrow \Rightarrow \xi_i \uparrow$ the representation

$$P\{\xi_S \le \xi_S^L\} \ge \alpha \qquad (2)$$

is the same as (1). If $y_i \uparrow \Rightarrow \xi_i \downarrow$, then the representation

$$P\{\xi_S \ge \xi_S^L\} \ge \alpha \qquad (3)$$

corresponds to (1). Generally, in case of a negative monotony, an upper bound of the constrained output induces a lower bound of the random variable and vice versa. No change between upper and lower bound will be in case of a positive monotone relation. This implies that the probability of holding the output constraint can be computed by integration in the corresponding region of the uncertain variable. It should be noted that all uncertain variables, which have an impact on y_i, have to be taken into account when computing $P\{y_i \le y_i^{SP}\}$. In addition, the values of the decision variables *u* have also an impact on the projected region. Then the bound ξ_S^L will change based on the realization of the individual uncertain variables $\xi_s, (s = 1, \cdots, S-1)$ and the value of *u*, i.e.

$$\xi_S^L = F^{-1}(\xi_1, \cdots, \xi_{S-1}, y_i^{SP}, u) \qquad (4)$$

and this leads to the following representation

$$P\{y_i \le y_i^{SP}\} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \int_{-\infty}^{\xi_S^L} \rho(\xi_1, \cdots, \xi_{S-1}, \xi_S) d\xi_S d\xi_{S-1} \cdots d\xi_1 \qquad (5)$$

Furthermore, for linking this method to a NLP framework, we need to compute the gradients of the output constraint probability to the decision variables *u*. From (4)-(5), *u* has the impact on the value of the probability through the integration bound of the corresponding region of the random inputs. Thus the gradients can be computed as follows:

$$\frac{\partial P\{y_i \le y_i^{SP}\}}{\partial u} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \rho(\xi_1, \cdots, \xi_{S-1}, \xi_S^L) \frac{\partial \xi_S^L}{\partial u} d\xi_{S-1} \cdots d\xi_1 \qquad (6)$$

The numerical integration of (6) can be computed simultaneously to (5).

For the numerical integration, collocation on finite elements is used. For this purpose the optimal number of collocation points and intervals need to be found in order to find a trade-off between computational time and accuracy. Recent studies have shown, that 5-point collocation is more efficient than 3-point-collocation at any rate. With two intervals, the error of probability computation is always less than 1%; with one interval, the error is at the worst between 1% and 2%.

Due to the model complexity, an explicit expression of (4) is usually not available. Therefore, a Newton-Raphson step has been used for steady state problems for computing the bound value ξ_S^L and its derivative with respect to u with given y_i^{SP}, u and $\xi_1,\cdots,\xi_{S-1}$ for each integrated subspace. However, for solving dynamic problems with a constraint variable $y_i^{SP}(t_f)$ for a fixed time point t_f and uncertain parameters occurring throughout the entire operation time with different u in different time intervals, a more general and efficient *dynamic solver* is required.

To be applicable to large scale dynamic problems in a reasonable computation time, the procedure of the dynamic solver can be divided into two steps:

1) Determination of the reverse projection of the feasible region by the bisectional method
2) Computation of the gradients $\frac{\partial \xi_S^l}{\partial u}$. The method is based on formulation of the total differential of the model equations $f(x,u,\xi)$:

$$df = \frac{\partial f}{\partial x}\frac{\partial x}{\partial u}du + \frac{\partial f}{\partial \xi_S^l}\frac{\partial \xi_S^l}{\partial u}du + \frac{\partial f}{\partial u}du = 0$$

Therefore a system of differential equations will be generated as follows:

$$\begin{bmatrix} J_1 & & & & & C_1 \\ A_2 & J_2 & & & & C_2 \\ & \ddots & \ddots & & & \vdots \\ & & A_i & J_i & & C_i \\ & & & \ddots & \ddots & C_{m-1} \\ & & & & A_m & J_m \end{bmatrix} \begin{bmatrix} x_{U,11} & \cdots & \cdots & x_{U,1m} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ x_{U,m1} & \cdots & \cdots & x_{U,mm} \end{bmatrix} = - \begin{bmatrix} F_1 & & & & \\ & F_2 & & & \\ & & \ddots & & \\ & & & F_i & \\ & & & & \ddots & \\ & & & & & F_m \end{bmatrix}$$

where J_i denotes the jacobian matrix $\left(\partial f/\partial x|_i\right)$ at time interval i and m is the number of time intervals. C_i is the gradient $\left(\partial f/\partial \xi_S^l|_i\right)$, A_i is $\left(\partial f_i / \partial x_{i-1}\right)$ and F_i signifies $\left(\partial f/\partial u|_i\right)$. The jacobian matrix at the last time interval J_m is adjusted by replacing the constrained variable with ξ_S^l. Thus, the desired gradient $\left(\partial \xi_S^l / \partial u\right)$ is included in the last line of the matrix, which denotes the gradients $\left(\partial x / \partial u\right)$. The unknowns in this DAE system, the values for x_U, will be computed using Gauss elimination.

The whole computational strategy for solving the nonlinear chance constrained optimization problem is a sequential NLP approach that can be depicted in Fig. 2. SQP is chosen for computing the values of the decision variables u in the NLP solver. The values of the objective function, the probabilistic constraints and their sensitivities are computed by the multivariate integration, while the upper and lower bounds of the integration region will be calculated through solving the model equations by the dynamic solver algorithm. It is worth noting that the computation of both the probability and the gradients is not limited to a certain kind of distribution form of the uncertain inputs, but works for any form of probability distribution.

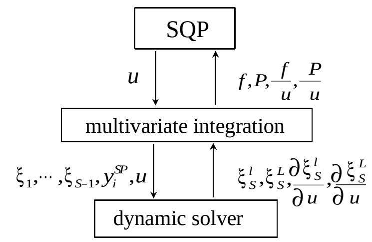

Fig. 2. Computational strategy for solving chance constrained problems

Joint chance constraints in nonlinear systems

To compute a joint constraint, again, there must be one uncertain variable ξ_S, which is monotone to all constrained output variables. Then this selected uncertain variable has to be defined as an upper or lower bound according to the bounds of the constrained outputs and the characteristics of the monotony as explained in the second section. In case, there are several constrained outputs inducing several upper or lower bounds, then for the integration of ξ_S the lowest possible value of the upper bound and the highest possible value of the lower bound is chosen. Thus, the joint probability concerning the output constraints will be formulated so that

$$P\left\{y_i \le y_i^{SP},\ i = 1,\cdots,I\right\} = P\left\{\xi_S^l \le \xi_S \le \xi_S^L\right\} \qquad (7)$$

where ξ_S^L and ξ_S^l are the upper and lower bound of the uncertain input region, respectively. This region is formed by the cutting planes mapped by $y_i(u,\xi) \le y_i^{SP}$, $(i = 1,\cdots,I)$. Then the joint probability (7) can be computed by:

$$P\left\{y_i \le y_i^{SP}, i = 1,\cdots,I\right\} = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\int_{\xi_S^l}^{\xi_S^L} \rho(\xi_1,\cdots,\xi_{S-1},\xi_S)\,d\xi_S\,d\xi_{S-1}\cdots d\xi_1 \qquad (8)$$

This formulation is applicable to all steady state problems, but also to dynamic processes, where the random variables are steady throughout the process. It should be noted, that if all constrained outputs have a positive monotone relation to the uncertain input, there will be no lower bound, but the lowest possible value will become the upper bound.

Application to reactive semibatch distillation

Batch processing is dynamic and provides a high degree of operational freedom. This new approach has been implemented for a complex industrial reactive semibatch distillation process, described by a rigorous model, which has been validated through a conventional batch run on the industrial site. A slightly endothermic trans-esterification of two esters and two alcohols takes place in the reboiler. During the batch a limited amount of educt alcohol will be fed to the reboiler to increase the reaction rate to the desired direction. The product alcohol (the lightest component) is distillated from the reboiler, through which the reaction will be shifted towards the product direction. It is assumed that the uncertainties are from the kinetic parameters (the activation energy and the frequency factor in the Arrhenius equation) and the tray efficiency η. The one uncertain variable, which is monotone to the restricted state variables in the probabilistic constraints at any rate is the tray efficiency η. That means there is a relation $\eta \uparrow \Rightarrow x_{D,1} \uparrow$ and also $\eta \uparrow \Rightarrow x_{A,NST} \downarrow$. According to (1)-(5) η^L can be used as the upper bound for the random variable η in the numerical integration of the probabilities $\overline{P}$ of the *complementary* event of the original constraints.

The actually wanted probability then will be found by $P = 1 - \overline{P}$. As an alternative, η^L could be the lower bound for computing the wanted probability. Thus, for given values of the restricted variables the corresponding tray efficiency η will be computed using the bisectional method starting with values for η between 0.1 and 0.96.

For the implementation we consider two cases, the simplified single fraction problem as case 1 and the more complex two-fraction problem as case 2.

Case 1: The single fraction problem:

The target of this optimization problem is the maximization of the total amount of distillate product ***J*** within a fixed time horizon and a fixed trajectory of feed flow rate of the educt alcohol. The product is restricted by a given purity specification of 0.99 mol/mol, which has to be formulated as a probabilistic constraint. Here the trajectory of the reflux ration is seen as the only independent variable to be optimized.

In Fig. 3 and table 1 the impact of different probability levels is illustrated, indicating the trade-off between the objective and robustness of the process. It can be noted, that mainly in the beginning time intervals, the probability level has an impact to the optimal process operation policy and thus only those time intervals are shown in Fig. 3.

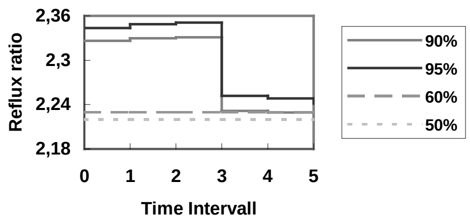

Fig. 3.impact of probability level to the reflux ratio

	50%	60%	90%	95%
J	0.2294831	0.2290534	0.2267549	0.2274652

Fig. 3: impact of probability level to the objective value

Case 2: The two-fraction problem

In the main cut period the product alcohol is accumulated in the first distillate accumulator with a given purity specification. At the end of the batch, a mixture of the product ester with a desired purity and the educt alcohol will be achieved in the reboiler and then separated by a recovery column.

The aim of the optimization is to minimize the batch operation time. Thus the independent variables of the problem are the feed flow rate *F* and the reflux ratio *Rv*. Considering the sequential approach, the nonlinear dynamic optimization problem is formulated as follows:

$$\min \; t_f \left(F(t), R_V, t_u, t_f\right)$$

$$\textbf{s.t.} \quad P\left\{x_{D,1}(t_{switch}) \geq 0.98 \; mol/mol\right\} \geq \alpha_1$$

$$P\left\{x_{A,NST}(t_f) \leq 0.002 \; mol/mol\right\} \geq \alpha_2$$

$$\int_{t_0}^{t_f} F(t)\,dt \leq 20 \; kmol \quad \text{and} \quad 0 \leq F(t) \leq 150 \; l/h$$

with $x_{D,1}$ and $x_{A,NST}$ as the average distillate composition at the end of the main cut period and the purity in the bottom, respectively. In order to handle the fraction switching-time t_{switch} and the total batch time t_f conveniently, the lengths of the different time intervals are also regarded as independent variables, additionally.

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