PROCESS OPTIMIZATION AND CONTROL UNDER CHANCE CONSTRAINTS

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Abstract: We propose to use chance constrained programming for process optimization and control under uncertainty. The stochastic property of the uncertainties is included in the problem formulation. The output constraints are to be ensured with a predefined confidence level. The problem is then transformed to an equivalent deterministic NLP problem. The solution of the problem has the feature of prediction, robustness and being closed-loop. In this paper, the basic concepts and solution strategies are discussed to illustrate the potential for optimization and control under uncertainty.

Keywords: uncertainty, chance constraints, linear, nonlinear, optimization, control

1. INTRODUCTION

It is a well-known fact that uncertainties exist in every chemical process. In most previous studies on process optimization and control, the stochastic properties of uncertainties have not been taken into account. In the industrial practice, uncertainties are compensated for by using conservative operating strategies, which may lead to considerably more costs than necessary. In addition, feedback control is used to compensate for uncertainties. However, compensation without considering the uncertainty properties is in fact the wait-and-see strategy and has several drawbacks. First, it is always *a posteriori*. Second, the system propagates the disturbances to connecting systems. Third, a feedback can not ensure constraints on open-loop variables. In many cases it is impossible to on-line measure some variables which describe product properties (e.g. composition, viscosity, density). These variables have to be open-loop under the uncertainties but they should be confined to a specified region corresponding to the product specifications.

To overcome these drawbacks, we have recently proposed and studied a new framework for process optimization and control under uncertainty. The uncertainty properties are to be included in the problem formulation. These properties can be gained by statistical analysis of historical data. A stochastic programming problem under chance constraints is formulated for both optimization and control. It will be relaxed to an equivalent deterministic NLP problem. The essential challenge lies in the computation of the probabilities of holding the constraints as well as their gradients. Approaches of chance constrained programming to linear, nonlinear and dynamic problems have been developed and applied to different process engineering problems. The method of moving horizon is employed for solving dynamic optimization and control problems under uncertainty.

While chance constrained programming has been applied in many disciplines like finance and management (Prekopa, 1995; Uryasev, 2000), few applications have been made in chemical process operations (Henrion et al., 2001). It has been used for batch process planning (Petkov and Maranas, 1997). Several studies on model predictive control using chance constrained programming have been carried out for linear processes (Schwarm and Nikolaou, 1999; Li et al. 2000 and 2002a,b). Recently, a method to nonlinear chance constrained problems was introduced for process optimization under uncertainty (Wendt et al., 2002). It has been extended to nonlinear dynamic optimization problems under uncertainty (Arellano-Garcia et al., 2003). In this paper, the basic principles of chance constrained programming and its applications to process optimization and control are discussed to illustrate its potential and limitation.

2. UNCERTAINTY ANALYSIS

In process operation, there are two general types of uncertainties. *External uncertainties* are from outside but have impacts on the process. They can be the rate and/or composition of feed and recycle flows as well as flows of utilities, the temperature and pressure of the coupled operating units or market conditions. *Internal uncertainties* represent the unavailability of knowledge of the process. For a determined model structure, they are uncertain model parameters often regressed from a limited number of experimental data. We call both of these *uncertain inputs*. Due to these uncertainties, conservative or aggressive decisions may be made. While internal uncertainties have been well studied in the framework of robust control in the past (Morari and Zafiriou, 1989; Kothare et al., 1996; Bemporad et al. 2002), external uncertainties have not been much emphasized.

As shown in Fig. 1, an uncertain input ξ can be constant (e.g. model parameters) or time-dependent (e.g. atmospheric temperature) in the future horizon $t \in [t_0, t_f]$. They are undetermined before their realization. The "realization" means either the measurable uncertain variables have been measured or parameters newly estimated. The distribution of the variables may have different forms. Very often normal (Gaussian) distribution is considered as an adequate assumption for many uncertain variables in the engineering practice. The basic justification of this statement is embodied in the central limit theorem (Maybeck, 1994). The values of mean and variance are usually available. The uncertain variables may be *correlated* or *uncorrelated*.

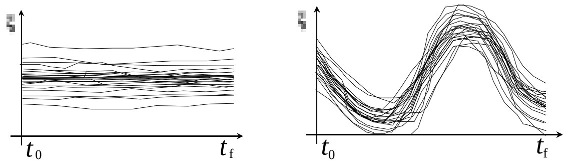

Fig. 1: Two different uncertain variables

These uncertain inputs will propagate through the process to output variables (e.g. temperature, composition). This makes the outputs also uncertain. A continuous process with constant uncertain inputs leads to a *steady-state* problem, while such a process with time-dependent uncertain inputs or a batch process is a *dynamic* problem under uncertainty. For a *nonlinear* process it is very difficult to analytically describe the distribution of the outputs. A scheme of *simulation* with sampling can address this problem. According to their distributions, random values are generated. After many runs of simulation with the sampled data, the probability distribution of the outputs can be gained. Besides Monte-Carlo, some efficient sampling strategies have been proposed (Diwekar and Kalagnanam, 1997). Obviously, the *wait-and-see* strategy can not result in satisfactory operations under these uncertainties. Thus we are confronted with making decisions *a priori* for the future operation (i.e. the *here-and-now* strategy). Under the uncertainties, a stochastic programming problem has to be defined and solved to answer these questions: 1) how to achieve an economically optimal operation? 2) how to ensure the constraints of the output variables? 3) how to prevent the propagation of the uncertainties to downstream processes? and 4) how to design a proper feedback control system?

3. CHANCE CONSTRAINED PROBLEMS

A general optimization or control problem under uncertainty can be formulated as

$$\begin{aligned} \min \quad & f(\mathbf{x},\mathbf{u},\boldsymbol{\xi}) \\ \text{s.t.} \quad & \mathbf{g}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\boldsymbol{\xi}) = \mathbf{0}, \quad \mathbf{x}(t_0) = \mathbf{x}_0 \\ & \mathbf{h}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\boldsymbol{\xi}) \geq \mathbf{0}, \\ & \mathbf{u}_{\min} \leq \mathbf{u} \leq \mathbf{u}_{\max},\ t_0 \leq t \leq t_f \end{aligned} \tag{1}$$

where *f* is the objective function, **g** and **h** are the vectors of equality and inequality constraints. **x, u** and $\boldsymbol{\xi}$ are the vectors of state, control and uncertain inputs, respectively. $\mathbf{x}_0$ is the known initial state. This dynamic nonlinear optimization problem has to be descretized with time intervals into a static problem so that it can be solved with the method of stochastic programming. Time-dependent uncertain inputs will be approximated as discretized uncertain variables in individual time intervals. In this work, they are assumed to have a correlated multivariate normal distribution.

There have been two general stochastic approaches (Kall and Wallace, 1994) to solve such problems. The *two-stage programming* uses recourse to deal with inequality constraints. The first-stage decision variables are determined and fixed before the realization of the uncertain variables, while the second-stage variables are decided after their realization. The violation of constraints is compensated for by some penalty functions and leads to additional costs for the second stage decisions. Since a proper penalty function is usually not available, the application of this method to operation and control may be not appropriate.

The other method is the *chance constrained programming*. Its unique feature is that the resulting solution ensures a predefined probability of satisfying the constraints. The solution will lead to an expected optimal value of the objective function by searching for the decision in a feasible region to hold a given confidence level, denoted as $\alpha\,(0 \leq \alpha \leq 1)$. Since α can be defined by the user, it is possible to select different levels and make a compromise between the function value and risk of constraint violation. It should be noted that with both solution strategies there have been, until now, no suitable approaches to nonlinear problems.

Recently, we have studied chance constrained programming for process optimization and control under uncertainty (Li et al. 2000 and 2002a,b; Henrion et al., 2001; Wendt et al., 2002). In engineering practice, a very popular form of inequality constraints is to specify or restrict some of *output variables* **y** (note **y** is part of **x**):

$$y_i^{\min} \le y_i(\mathbf{u},\xi) \le y_i^{\max} \quad i = 1,\cdots,I \tag{2}$$

$y_i^{\min}, y_i^{\max}$ are the required lower and upper bound of an output, such as a pressure or a temperature restriction of a plant. Holding these constraints is usually critical for the production and safety. For $t \in [t_0, t_f]$ a probabilistic form of (2) is

$$\Pr\left\{ y_i^{\min} \le y_i(\mathbf{u},\xi) \le y_i^{\max},\ i = 1,\cdots,I \right\} \ge \alpha \tag{3}$$

With this representation, all inequalities are included in the probability computation. It means that they should be satisfied simultaneously with the given probability. This is called *joint* probabilistic (chance) constraint. Another form is *single* chance constraint, where individual probabilities of ensuring each inequality will be held:

$$\Pr\left\{ y_i^{\min} \le y_i(\mathbf{u},\xi) \le y_i^{\max} \right\} \ge \alpha_i,\ \ i = 1,\cdots,I \tag{4}$$

It should be noted that in deterministic approaches the expected values of the uncertain variables are usually employed. In reality, however, the uncertain variables will deviate from their expected values. Thus the implementation of the results from a deterministic approach will violate the inequality constraints with a probability of around 50%. The difference between (3) and (4) is that a joint chance constraint requires the reliability in the output feasible region as a *whole*, while single chance constraints demands the reliability in the *individual* output feasible region. If the constraints are related to the safety consideration of a process operation, a joint chance constraint may be preferred. Single chance constraints may be used when some output constraints are more critical than the other ones. The equalities in (1) are the model equations of the process. They have to be satisfied with any realization of the uncertain variables. In fact, the effect of the model equations is a projection of the space of the random variables ξ as inputs to a space of state variables **x**, with given controls **u**. Thus the equalities will be eliminated if an integration of the equations in the space of the uncertain variables is made. It implies that a sequential approach is suitable for solving stochastic problems with equality constraints. To treat the objective function in (1), minimizing the expected value and the variance of the objective function has usually been adopted (Darlington et al. 1999):

$$\min\ \ \mathrm{E}\left[f(\mathbf{x},\mathbf{u},\xi)\right] + \omega\, D\left[f(\mathbf{x},\mathbf{u},\xi)\right] \tag{5}$$

E and D are the operators of expectation and variation, respectively. ω is a weighting factor between the two terms. In the sense of relaxation the objective function in (1) is now a deterministic function through these two operators. Now a general chance constrained problem is formulated with (5) as objective function and (3) or (4) with constraints.

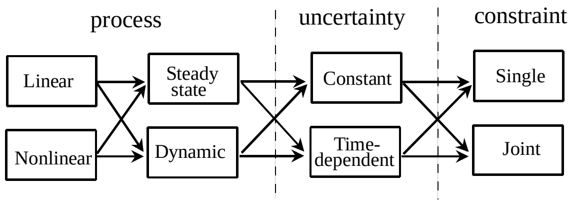

Fig. 2: Classification of chance constrained problems

As shown in Fig. 2, such problems can be classified based on the properties of processes, uncertainties and constraint forms. Thus there are 16 different formulations. We can use the initial letters to denote the problems. For example, a steady state process with constant uncertainties under single chance constraint is called an LSCS problem. It is interesting to note that LSTS and NSTS can be solved separately for each interval, while for LSTJ and NSTJ (a quasi-dynamic problem) the whole time horizon should be considered. To solve such problems with an existing optimization routine, the probability of holding the constraints has to be computed. Moreover, the gradients of the probability function to the controls are required. Different problems have different degrees of complexity for computing these values, which will be discussed in the following two sections.

4. APPROACH TO LINEAR SYSTEMS

Chance constrained linear problems can be relatively easily treated and have some nice properties. Theoretical results show that the feasible region of linear problems with quasi-concavely distributed uncertain variables is convex (Prekopa, 1995). Another merit property is that linear transformations of multivariate normally distributed variables have the same distribution. Optimization of linear steady state systems (LSCS and LSCJ) under constant uncertain variables has been well studied (see Kall and Wallace). It can be applied in process design and planning under uncertainty.

We consider *linear dynamic* systems with *time dependent* uncertain inputs (LDTS and LDTJ). The outputs in the future horizon depend on the current state, the future and past controls as well as uncertain inputs. The uncertain inputs include both uncertain parameters (e.g. step response coefficients) and disturbances. The controls in the horizon will be decided to optimize some objective function and ensure the chance constraints for the outputs. A quadratic objective function leads to a chance constrained *model predictive control*, as shown in Fig. 3. One can easily notice that the novelty of this controller, compared with the conventional MPC, is it includes the uncertainties *explicitly* in the problem formulation. Moreover, it is worth noting that the objective function may only include the quadratic terms of controls, since the outputs are confined in the chance constraints, e.g.

$$\min \sum_j \sum_l \omega_l [u_l(t+j) - u_l(t+j-1)]^2 \qquad (5)$$

For linear MPC with *single* chance constraints (LDTS), the chance constraints can easily be transformed to linear deterministic inequalities. It leads to a QP problem and thus the solution can be derived analytically (Schwarm and Nikolaou, 1999).

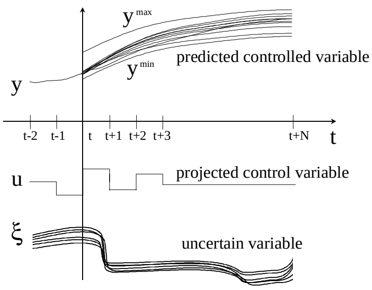

Fig. 3: Chance constrained MPC

In cases of problems with a *joint* chance constraint (LDTJ), an explicit solution cannot be obtained, since the calculation of a joint probability of multivariate uncertain variables is needed. Although one chance constraint for all outputs and all time points can be formulated, it is natural to constrain each output separately, i.e. for $i = 1, \cdots, I$

$$\Pr\{y_i^{\min}(t+j) \le y_i(t+j) \le y_i^{\max}(t+j),\ j = 1, \cdots, N\} \ge \alpha_i \qquad (6)$$

Note that even if the uncertain inputs are uncorrelated, the outputs are correlated through the linear propagation. With some linear transformation, (6) can be described as the following form

$$\Pr\{\boldsymbol{\xi}_i' \le \mathbf{A}_i \mathbf{u} + \mathbf{b}_i\} \ge \alpha_i \qquad (7)$$

$\boldsymbol{\xi}_i'$ is an *N*-dimensional uncertain vector. The joint probability makes (7) nonlinear constraints and the stochastic MPC becomes an NLP problem. Unfortunately, it is not possible to easily compute those probability values even numerically, if the dimension is larger than 3. A simulation scheme to estimate joint probabilities was proposed (Prekopa (1995). The first and second term of the inclusion-exclusion formula are computed exactly and the rest terms are evaluated by sampling. Moreover, the gradient calculation is required to solve the problem with an NLP solver, which is more difficult. We used this simulation scheme for the probability computation and proposed a reduced gradient computation strategy (Li et al., 2000, 2002a). The efficient sampling by Diwekar and Kalagnanam (1997) is used. SQP is used for the optimization and the control proceeds by moving horizon. After the control of the first time interval is implemented, together with the realization of the uncertain inputs in this interval, the system moves to the new state, and the control policy in the new horizon will be computed. The tuning parameters of this algorithm are the length *N* of the time horizon and the confidence level α. As a kind of predictive controller a large *N* is desired, but the computation time will be greater. The major computation load is due to sampling of the uncertain variables to evaluate the probabilities and their gradients. A larger *N* means more uncertain variables are included in the problem formulation.

Tuning the value of α is an issue of the relation between *feasibility* and *profitability*. Of course a high confidence level to ensure the constraints is always preferred. The solution of a defined problem, however, is only able to arrive at a maximum value $\alpha^{\max}$ which is dependent on the properties of the uncertain inputs and the restriction of the controls and outputs. The knowledge of $\alpha^{\max}$ is crucial; if a value greater than $\alpha^{\max}$ is chosen, the feasible region will be empty. An easy-to-use method was proposed to compute this maximum value for SISO systems (Li et al., 2002b) which can be extended to MIMO systems. The basic idea is to map the stochastic inputs to outputs and analyze the property of the outputs. It can be proved that the joint probability has the maximum value if the mean values of the outputs are at the middle of their restricted region $[y^{\min}, y^{\max}]$. Thus $\alpha^{\max}$ can be obtained via a simulation run. The *profitability* of the stochastic MPC means the achievability of the objective function value, which is also a function of the confidence level. They have a monotone relation: the value of objective function will be degraded if α is increased. One can analyze the profile of the function value with changing α and decide on a suitable trade-off between profitability and reliability.

5. APPROACH TO NONLINEAR SYSTEMS

The motivation to consider nonlinear chance constrained problems is to find systematic ways to compensate for uncertainties so as to avoid intuitive or empirical decisions. Recently we proposed a solution method to nonlinear *steady state* problems under *single* chance constraints (NSCS), in which direct computation of the probability of holding the output constraints is avoided (Wendt et al., 2002). The basic idea is to map the chance constrained region of the outputs back to a bounded region of the uncertain inputs. This can be done by a monotone relationship between an input ξ_S (assuming there are S uncertain variables) and the constrained output y_i. Thus the output probability can be computed by integration of the density function of the uncertain inputs, e.g. if $\xi_S \uparrow \Rightarrow y_i \uparrow$, then

$$\Pr\{y_i \le y_i^{\max}\} = \Pr\{\xi_S \le \xi_S^{\max}, \forall \xi_1, \cdots \xi_{S-1}\} = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\xi_S^{\max}} \rho(\xi_1, \cdots, \xi_S) d\xi_S \cdots d\xi_1 \qquad (8)$$

For the multivariate integration, collocation on finite elements is used to discretize the bounded region of the uncertain inputs. The input boundary $\xi_S^{\max}$ is computed inversely by the Newton-Raphson method based on the output value of $y_i^{\max}$. Since this boundary depends on the realization of the uncertain variables ($\xi_1, \cdots \xi_{S-1}$), it has to be computed on each collocation point of these variables. In this way, the equality constraints (model equations) are eliminated by expressing the state variables in terms of decision and uncertain variables. Again, a sequential solution approach is used. It can principally be described with Fig. 4. Due to the uncertainty, three different controls will result in three different output distributions: 1) too conservative (e.g. resulting in great operation costs), 2) acceptable and 3) too aggressive (resulting a high probability of constraint violation). Due to the monotony, the bound values ($\xi_i^{\max(1)}, \xi_i^{\max(2)}, \xi_i^{\max(3)}$) of the uncertain variable can be determined and thus the probabilities of holding the constraint can be computed.

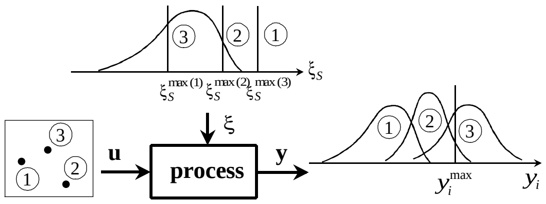

Fig. 4: Approach to nonlinear constrained problems

Principally, this approach can solve problems under uncertainties with any kind of distributions, provided the density function and a monotone relationship between the constrained variable and one of the uncertain inputs are available. A numerical integration scheme for problems with correlated Gaussian inputs is developed. It should be noted that for normal distributions the boundaries of the infinite integrals in (8) can be chosen as $[-3\sigma, 3\sigma]$. A nested computational scheme to the multivariate integration is proposed based on the fact that the S-dimensional integration can be computed by an (S-1)-dimensional integration. The gradients of the probabilities to the controls can be computed in the same way. To address the issue of feasibility, one can first define the objective function as maximization of the achievable probability. The problem is then solved for the value of $\alpha^{\max}$. For some practical processes, one may gain this value through simulation. For example, if the control is monotone with the constrained variable, then $\alpha^{\max}$ corresponds to the confidence level with the lower or upper bound of this control variable. This approach can straightforwardly be extended to multiple single probabilistic constraints. For each constraint a probability computation will be made in the form of (8). In this case, different confidence levels can be selected for different output constraints. The extension of the approach to a joint chance constrained problem (NSCJ) is not a trivial task, since it may be difficult to find an uncertain variable which is monotone with the joint probability. It may be possible to find such a variable by carefully analyzing the relations between the uncertain inputs and constrained outputs. This can be done with process simulation by perturbing the uncertain variables.

This approach has been extended to solve NDCS problems of nonlinear dynamic optimization under uncertainty (Arellano-Garcia et al., 2003). We consider dynamic problems with constrained outputs at selected time points and with constant uncertain inputs. The control policy $u(t)$ for the entire operation time will be developed to optimize the objective function subject to single chance constraints of holding the point restrictions. This is a suitable formulation to optimize batch process operations under model parameter uncertainty. Two difficulties have to be overcome in solving such dynamic problems. First, since multiple time intervals are considered, the reverse projection of the output feasible region to a region of uncertain inputs is not trivial. The method of bisection through simulation seems to be efficient to address this problem. This is because it is a one-to-one projection. Second, since the controls have different impacts on the outputs in different time intervals, the gradients of the uncertain input to the controls in each interval have to be computed and passed to the time points from interval to interval in order to compute the gradients of the probability.

6. OPEN-CLOSED FRAMEWORK

A closed-loop control requires on-line measured values of controlled variables. However, many variables in the engineering practice can not be measured on-line (e.g. concentration, viscosity, density etc.). These variables represent the qualities of products and their control is desired. To address this problem, measurable variables (temperature, pressure) are chosen as controlled variables to indirectly control the product quality. This concept can be described with Fig. 5. **y** will be controlled at their setpoints $\mathbf{y}^{SP}$ by using controls **u**. Control of $\mathbf{y}^{C}$ is desired, but due to the lack of on-line measurement it has to be open-loop. In these cases,

$\mathbf{y}^C$ needs to be constrained but **y** is not constrained. To ensure the product quality, the present solution in the industrial practice is to choose an extremely conservative setpoint value. This leads to the fact that the product quality will unnecessarily be much higher than specified and, due to the greater flow rates of the controls, the operation costs will be much higher than necessary.

Therefore, it is necessary to choose an optimal set of setpoints for the controllers. This can be gained by chance constrained optimization, i.e. the costs will be minimized and the constraints to $\mathbf{y}^C$ satisfied with a desired confidence level. This leads to a new concept of control: to control open loop processes by closed-loop control. Unlike the above problem definitions where controls are decision variables, in the closed framework the setpoints of the measurable outputs should be defined as decision variables. Moreover, controller equations have to be included in the problem formulation. It is normally a complicated NDTS or NDTJ problem. In practice, many continuous processes have constant uncertain inputs, and their impact on the controlled variables **y** can easily be compensated for by the controllers. Then the problem is reduced to a NSCS or NSCJ problem which can be solved by the approach discussed in the last section.

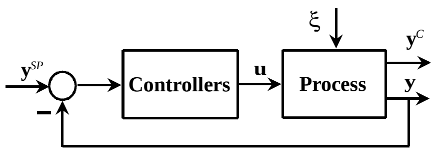

Fig. 5: The open-closed framework

The approach has been applied in a pilot distillation column to separate a methanol-water mixture with uncertain feed flow and composition as well as column pressure (Li et al. 2003). The operating energy is to be minimized subject to a rigorous model composed of component and energy balances, vapor-liquid equilibrium and tray hydraulics for each tray. The temperatures on the sensitive trays are selected as the controlled variables, while the bottom and top product purity are probabilistically constrained. The optimization results provide the profiles of the objective function value and the corresponding controller setpoints along with the confidence level to hold the product specification.

7. CONCLUSIONS

We have discussed the concepts, solution strategies and perspectives of chance constrained optimization and control. Since the uncertainty properties are taken into account, the solution of the problem is a decision *a priori*. A predefined probability to satisfy the constraints will be held under the uncertainty and thus the decision is robust. Moreover, the solution provides a comprehensive relationship between the performance criterion and the probability level of satisfying the constraints. Thus one can decide on proper actions which will result in a desired compromise between profitability and reliability. In this way, conservative or aggressive decisions, which may have been made so far, can be prevented. We have solved LDTJ, NSCS and NDCS problems and applied these approaches to several optimization and control applications. Development of more efficient methods to address high dimension NDTJ problems remains a challenge for future work.

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