Chance Constrained Programming Approach to
Process Optimization under Uncertainty

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Abstract
Deterministic optimization approaches have been well developed and widely used in the process industry to accomplish off-line and on-line process optimization. The challenging task for the academic research currently is to address large-scale, complex optimization problems under various uncertainties. Therefore, investigations on the development of stochastic optimization approaches are necessitated. In the last few years we proposed and utilized a new solution concept to deal with optimization problems under uncertain operating conditions as well as uncertain model parameters. Stochastic optimization problems are solved with the methodology of chance constrained programming. The optimization problem is relaxed into an equivalent nonlinear optimization problem such that it can be solved by a nonlinear programming (NLP) solver. The major challenge towards solving chance constrained optimization problems lies in the computation of the probability and its derivatives of satisfying inequality constraints. Approaches to addressing linear, nonlinear, steady-state as well as dynamic optimization problems under uncertainty have been developed and applied to various optimization tasks with uncertainties such as optimal design and operation, optimal production planning as well as optimal control of industrial processes under uncertainty. An overview on the theoretical development and practical applications in our recent work will be presented.

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

1. Introduction
The research in the area of process optimization under uncertainty has been initiated by Grossmann and his coworkers (see Bansal et al., 2002). The emphasis in previous studies has mainly been on process design under uncertainty. Most studies follow the definition of feasibility test (Halemane and Grossmann, 1983) and flexibility index (Swaney and Grossmann, 1985a,b), in which uncertain variables over certain intervals are considered. A nested two-stage approach was proposed to solve the optimization problem (Grossmann and Floudas, 1987; Pistikopoulos and Ierapetritou, 1995; Rooney and Biegler, 2003). Using these approaches, the optimality and reliability will be ensured by a conservative decision. The iteration between the first and second stage to solve the problem demands more expensive computational efforts. The violation of constraints is compensated by some penalty functions and leads to additional costs for the second stage decision. This approach is appropriate to solve planning problems under demand uncertainty (Petkov and Maranas, 1998). Furthermore, the solution with the compensation method provides no obvious information on the relation between reliability and probability which is crucial in decision making.
In the industrial practice, an overestimation of uncertainties, which is a widespread practice in the chemical industry, leads to a conservative decision resulting in an unnecessary deterioration of the objective function. The main reason for these intuitive decisions in planning chemical process operations is due to the lack of systematic reliability analysis. In other cases, an aggressive decision may be preferred due to profit expectations. This strategy will probably lead to constraint violations as a consequence. Accordingly, a systematic way is required to evaluate the trade-off between profitability and reliability. The implication of conservative and aggressive operations is illustrated in Fig. 1a, showing the distribution of a constrained output variable. Chance constrained programming is a competitive tool for solving optimization problems under uncertainty. Its main feature is that the resulting decision ensures the probability of complying with constraints, i.e., the confidence level of being feasible. Thus, using chance constrained programming the relationship between the profitability and reliability can be quantified. In other words, the solution of the problem provides comprehensive information on the economical achievement as a function of the desired confidence level of satisfying process constraints. In the last few years, we have developed approaches of chance constrained programming to linear, nonlinear and dynamic problems and applied to different process engineering problems.

2. Optimization under uncertainty
Uncertainties can be generally divided into external uncertainties like feed rate and/or its composition recycle flows, temperature and pressure of the coupled operating units, supply of raw material and utilities, customer demand, prices, market conditions. Internal uncertainties represent the unavailability of process knowledge such as model parameters. Model parameters are often regressed from a limited number of experimental data. While internal uncertainties have been well studied, external uncertainties have not been much emphasized. Moreover, they can be constant or time-dependent. Usually the distribution of an uncertain variable can be gained through statistical regression from previous available data or through interpolation or extrapolation. There has been an explosive growth of computer-based process monitoring systems, which makes it relatively easy to acquire process data to be utilized for distribution analysis. Uncertain variables may be correlated or uncorrelated and their stochastic distribution may also have different forms. Often normal (Gaussian) distribution is considered as an adequate assumption for many uncertain variables in the engineering practice. The values of mean and variance are usually available. These uncertain input variables will propagate through the process to the output variables and the outputs will also be uncertain. For a nonlinear process it is very difficult to analytically describe the distribution of the outputs. The basic idea of optimization under uncertainty is to integrate the available stochastic information into the optimization problem formulation.
3. Chance constrained optimization

A general chance constrained optimization problem can be formulated as follows:

\[
\begin{align*}
\text{min} & \quad E[f(x, u, \xi)] + \omega \ D[f(x, u, \xi)] \\
\text{s.t.} & \quad g(x, u, \xi) = 0 \\
& \quad \Pr\{h(x, u, \xi) \geq 0\} \geq \alpha \quad x(t_0) = x_0
\end{align*}
\]

where \( f \) is the objective function, \( E \) and \( D \) are its expected value and variance, respectively. The vectors \( g \) and \( h \) represents the equality (model equations) and inequality constraints. \( x, u \) and \( \xi \) are the vectors of state, control and uncertain parameters. \( \Pr\{h(x, u, \xi) \geq 0\} \) represents the reliability of complying with the inequality constraints \( h \), while \( \alpha \) is the user-predefined confidence level (0 to 1). There are two forms to define the chance constraints: single or joint. In the former, constraints are satisfied individually, while the latter requires them to be fulfilled simultaneously. Based on the process properties, uncertainties, and constraint forms, chance constrained problems can be formulated in 16 different types of problems (Fig. 1b). The resulting problem will then be relaxed to an equivalent nonlinear programming (NLP) problem. The main challenge in solving such problems lies in the computation of probabilities of holding the constraints as well as their gradients.

3.1. Solution approaches

3.1.1. Linear systems

The main feature of chance constrained linear problems is that, resulting from linear transformations, outputs have the same distribution as uncertain inputs. Theoretical results show that the feasible region of linear problems with quasi-concavely distributed uncertain variables is convex (Prekopa, 1995). Optimization of linear steady state systems under constant uncertain variables has been well studied (Kall and Wallace, Li et al., 2003, 2004). It can be applied in process design and planning under uncertainty. We have considered linear dynamic systems with time dependent uncertain inputs. 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 and disturbances. In the case of a linear system with single chance constraints, chance constraints can be easily transformed to linear deterministic inequalities. It leads to a QP problem and thus the solution can be derived analytically (Schwarm and Nikolaou, 1999, Li et al., 2002). In cases of problems with a joint chance constraint, an explicit solution cannot be obtained, since the calculation of a joint probability of multivariate uncertain variables is needed. It should be noted that even if the uncertain inputs are uncorrelated, the outputs are correlated through the linear propagation. With a joint probability the optimisation problem becomes an NLP problem. Unfortunately, it is not possible to easily compute the probability value even numerically, if the dimension is larger than 3. We used the simulation scheme proposed by Prekopa (1995) for the probability computation and proposed a reduced gradient computation strategy (Li et al., 2000, 2002a). Here an efficient sampling approach proposed by Diwekar and Kalagnanam (1997) is used in these computations.

3.1.2. Nonlinear systems

Due to the nonlinear propagation, it is difficult to gain the stochastic distribution of output variables. Thus, nonlinear chance constrained programming remained as an unresolved problem. The solution strategy to nonlinear stochastic programming under
chance constraints is also to adopt a relaxation to transform it into a deterministic NLP problem. The essential challenge here lies in the computation of probabilities of holding constraints as well as their gradients. A computation method for one single probabilistic constraint is proposed by Wendt et al. (2001). The basic idea of this method is to map the uncertain output distribution to that of the uncertain input variables. For this purpose, an uncertain variable $\xi_s$, which has a monotonic relationship with the output constrained variable $y^C$, is to be found. Due to the monotony, the boundary of the constrained value $y^{\text{Bound}}_C$ in the output region corresponds to a limit value $\xi^L_s$ for $\xi_s$ within the input region. This limit value can be computed by solving the model equations with given decision variables $u$ and the boundary value $y^{\text{Bound}}_C$. Then, the probability computation of the output constraints can be transformed to a multivariate integration in the limited area of uncertain inputs:

$$P\{y^C \leq y^{\text{Bound}}_C\} = P\{\xi_s \leq \xi^L_s, \xi_s \in \mathbb{R}^s, s \neq k\} = \int_{-\infty}^{\xi^L_s} \cdots \int_{-\infty}^{\xi^L_s} \rho(\xi_1, \ldots, \xi_k) d\xi_1 \cdots d\xi_k$$  \hspace{1cm} (2)

where $\rho(\xi)$ is the unified distribution function of $\xi$. For the multivariate integration, we use collocation on finite elements to discretize the bounded region of the uncertain inputs. The input boundary $\xi^L_s$ is computed by the Newton-Raphson method based on the output value of $y^{\text{Bound}}_C$. Since this boundary depends on the realization of the uncertain variables $(\xi_1, \ldots, \xi_{s-1})$, 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. This solution strategy is not dependent on the distribution of the uncertain variables, if the multivariate integration in (2) can be carried out. This procedure of probability computation can be straightforwardly extended to the multiple single probabilistic constraints. However, the extension of the probability computation procedure to a joint probabilistic constraint is not a trivial task, since it is difficult to find an uncertain variable which is monotone to all outputs. A crucial issue in dealing with probabilistic constraints is the convexity analysis of the problem for nonlinear systems. An analytical result concerning this issue is given by Prékopa (1995). It states that if the constraints form a convex set and if the density function is logarithmically concave, the corresponding problem may be convex. Many but not all of the usually existing distributions share the property of a log-concave density, e.g. multivariate normal distribution or uniform distribution on bounded convex sets (Henrion et al., 2001).

### 3.1.3. Nonlinear dynamic systems

The chance constrained approach has been extended to solve problems of nonlinear dynamic optimization under uncertainty (Arellano-Garcia et al., 2003). The approach involves efficient algorithms for realizing the required reverse mapping from the uncertain constrained output to the uncertain input. In the probability and gradient computation an optimal number of collocation points is chosen so that the original idea is applicable for dynamic optimization problems with larger scale. Furthermore, the analysis of the impact of the probability limits of the chance constraints on optimal process operation policies, particularly with regard to the optimized value of the objective function, is an important issue. Thus, an efficient search algorithm of the lower and upper bounds of the uncertain input with regard to the integration of the probability density function, and an efficient approach to gradient computation have been developed to deal with both single and joint probabilistically constraints (Arellano-Garcia et al., 2003). The joint probabilistical constraint is generally more severe than
single constraints with the same limit since it describes the satisfaction of all restrictions simultaneously.

3.2. Applications
Probabilistic programming has been applied in many disciplines like finance and management. However, very few applications have been made in chemical process design and operations. In the past years, we have implemented our chance constrained solution approaches to address different process engineering problems. We deal with production planning problems under uncertain market conditions (Li et al., 2003, 2004) as well as refinery planning under uncertain demand (Li et al., 2004). The problems can be formulated as a dynamic mixed-integer chance constrained optimization problem which can be relaxed to an equivalent deterministic MILP formulation. An optimal decision with a desirable trade-off can be made for the future purchase, sales and operation. The stochastic dynamic optimization approach has been successfully implemented for a reactive batch distillation process with single and joint constraints (Arellano-Garcia et al., 2003).

4. Process control under Uncertainty
Feedback control systems are used in unit operations to follow the decided operating point. However, many important process variables are not closed-loop controlled. This fact leads to an alternative concept of control based on chance constraints. We proposed a robust control strategy, model predictive control under chance constraints, to deal with multivariable constrained control problems. Both model and disturbance uncertainties are considered and assumed to be correlated multivariate stochastic variables. The output constraints are to be held with a predefined probability with respect to the entire horizon. The problem formulated is a stochastic program under joint probabilistic constraints. Using an efficient sampling method this problem is relaxed to a nonlinear programming problem which can be solved by SQP. Simulation results of a distillation column control show the performances of the proposed strategy (Li et al., 2000). Under the assumption of a linear system, the formulated problem is convex. Thus, it can be solved with a nonlinear programming solver. Probability values and gradients of satisfying constraints, composed of disturbance sequences with multivariate normal distribution, are computed with an efficient framework (Li et al., 2002, 2004). Unlike the linear case in which controls only affect the mean of the outputs, for nonlinear processes they have impact on both mean and covariance of the outputs. A mixing process with both uncertain feed flow rate and uncertain feed composition was used to illustrate the effectiveness of chance constrained nonlinear MPC (Xie et al., 2005). To realize the feedback control, the operating policy is adjusted from period to period based on the moving horizon approach.

5. Concluding remarks
An overview on the theoretical development and practical applications of chance constrained programming is presented. Our contribution to process optimization under uncertainty is that the solution results from the approaches developed can provide both optimal and reliable decisions for process design and operation. Moreover, analysis of the results makes it possible to identify the critical constraint which cuts off the largest part of the feasible region. This is a piece of important information for the decision-maker to relax the constraint, if necessary, so as to gain a meaningful decision. It is foreseeable that probabilistic programming will be a promising technique in solving optimization problems under uncertainty in the process industry.
References


