Chance Constrained Optimization of Process Systems under Uncertainty

PhD Thesis by Harvey ARELLANO-GARCIA

Summary

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 is currently to address large-scale, complex optimization problems under various uncertainties. Therefore, investigations on the development of stochastic optimization approaches are required. In this Thesis, a new approach for chance constrained programming of large-scale nonlinear dynamic systems under uncertain operating conditions as well as uncertain model parameters is presented. The stochastic property of the uncertainties is explicitly considered in the problem formulation in which some input and state constraints are to be complied with predefined probability levels. The method considers a nonlinear relation between the uncertain input and the constrained variables. The resulting optimization problem is then 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. The formulation of single or joint probability limits incorporates the issue of feasibility and the contemplation of trade-off between robustness and profitability regarding the objective function values. The new approach is relevant to all cases when uncertainty can be described by any kind of joint correlated multivariate distribution function.

The potential and the efficiency of the presented systematic methodology are illustrated with application to different processes under uncertainty, in particular, transient processes. Moreover, the functionality and efficiency of the developed chance constrained framework are demonstrated throughout on examples of design, operation and control problems. Besides, two model-based approaches are developed to provide a close integration of dynamic real time optimization D-RTO and control, and to cope with uncertainty.

Problem Statement

Robust decision making under uncertainty is deemed to be a crucial factor in many discipline and application areas. The competitive nature of the market environment imposes reliability requirements in meeting product demands and quality standards. The chemical industry is, therefore, required to make design and operating decisions which satisfy several conflicting goals in an optimal and safe manner. However, uncertainty and variability are inherent characteristics of any process system. They arise due to the unpredictable and instantaneous variability of different process conditions, such as temperature and pressure of coupled operating units, market conditions, (recycle) flow rates and/or compositions or other model parameters such as kinetic constants or equilibrium parameters. These uncertainties or disturbances are often multivariate and form correlated stochastic sequences which have a chain-effect on each unit operation of a production line.

In industrial practice, uncertainties are usually compensated for by using conservative measures such as over-design of process equipment and then retrofits to overcome operability bottlenecks, or overestimation of operational parameters caused by worst case assumptions of the uncertain parameters, which leads to a significant deterioration of the objective function in an optimization problem. In other deterministic approaches, the expected values are used, which most likely leads to violations of the constraints when the decision variables are implemented on site. Moreover, using feedback control to compensate the uncertainty effects can not ensure adherence to the constraints on the open-loop variables. In several cases, particular variables describing product properties like composition, viscosity, density, and etc. can not be measured online. These variables are open-loop under the uncertainties, but they are supposed to be confined to a specific region corresponding to the product specifications. It should be noted that even measurable disturbance variables are also stochastic variables, because they may have been measured to the present time point, but their future values are unknown. However, in conventional design methods for feedback control systems the description of disturbances is not rigorous. Step change and white noise are the two types of disturbances typically considered thus far. Consequently, the consideration of uncertainties/disturbances and their stochastic properties in optimization approaches are necessary for robust process design, operation, and control.

In this thesis, the main focus is related to the application to transient processes. The optimization of such inherent dynamic processes is usually performed using model-based optimization techniques. In most previous studies, a nominal model is considered, with which the outcomes of a deterministic optimization allow neither variation nor uncertainty on operating conditions or model parameters. Moreover, it is not possible to generate highly accurate phenomenological models for most chemical processes because of the imprecise values of their physical parameters, and the lack of complete understanding of the underlying physical phenomena. The usually limited quality and quantity of input-output data used to fit the model implies that the model will not be an exact representation of the real process. Thus, the practical implementation of model-based techniques often leads to a significant discrepancy between reality and simulation. Therefore, the existence of these uncertainties has a detrimental impact on the optimized process and raises questions like: ***what would be the probability of complying with the constraints in accordance with the optimized operating policy?*** Handling uncertainty, which becomes important especially in the presence of constraints on quality and safety, has not been adequately addressed so far and constitutes a significant bottleneck in applying optimization techniques to real processes. Therefore, accounting for the uncertainties involved in an optimization problem formulation, any improvement obtained regarding a specified economic objective function may occasionally become irrelevant, i.e. safety, reliability, and operability are often decisive, and more crucial than an economic objective (Grossmann and Morari, 1984). However, these issues are more complex and there is no obvious approach to suitably assess them (Figure 1). Thus, in most cases, conservative decisions based on heuristics or empirical rules are made which might lead to a substantial profit decrease. Accordingly, it demands systematic methods to evaluate the trade-off between profitability and reliability of a planned operation.

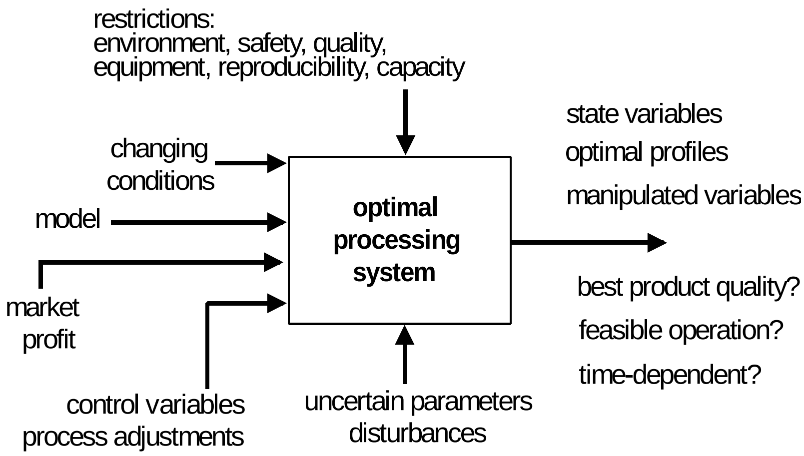

Figure 1: General operational objective targets.

State of the art

During the past decades several approaches have been suggested to address these problems in a systematic manner. These techniques mostly differ in how uncertainty is handled as well as in the objectives that may include process flexibility, profitability, and/or robustness. In general, the direct solution can be problematic due to the difficulty in both evaluating the integral over the uncertain parameter space and ensuring feasibility of the inequalities for all parameter values instances (Samsatli et al., 1998). Overview of developments in the area of process design and operations under uncertainty are given in comprehensive reviews of Grossmann et al. (1983), Kall and Wallace (1994), Pistikopoulos (1995), Wets (1996), Diwekar (2003), Sahinidis (2004). The emphasis of these studies, particularly in chemical engineering, has been mainly on process design problems. While most of the researchers were concerned about independent uncertain variables, Rooney and Biegler (1999, 2001) studied the effect of correlated uncertain variables on plant design. Two approaches have been used to represent uncertain variables: discrete and continuous distribution. In the former, the bounded uncertain variables are discretized into multiple intervals such that each individual interval represents a scenario with an approximated discrete distribution (Halemane and Grossmann, 1993; Subrahmanyam et al., 1994; Pistikopoulos and Ierapetritou, 1995; Rooney and Biegler, 1999). Thus, so-called multiperiod optimization problems are formulated. The second approach considers the continuous stochastic distribution of the uncertain variables, in which a multivariate numerical integration method will be chosen. This leads to a stochastic programming problem. An approximated integration through a sampling scheme (Diwekar and Kalagnannam, 1997) and a direct numerical integration (Bernado et al., 1999) have been used. Alternatively to sampled optimization algorithms, the stochastic problem can be relaxed to an equivalent NLP problem and then solved by using standard techniques. Thus, the optimization problem needs to be reformulated. If the uncertain variables have an impact on the objective function, it is usually formulated as the expected value of the objective function (Torvi and Herzberg, 1997; Acevedo and Pistikopoulos, 1998). Practically most of the previous cited works employed the two-stage programming method with the recourse formulation to deal with inequality constraints. In the two-stage approach, the first-stage decision variables are predetermined before the realization of the uncertain variables, while the second-stage variables are decided after their realization. Moreover, in the recourse formulation, violation of the constraints is allowed, but penalized through penalty terms in the objective function. This leads to additional costs regarding the second-stage decisions. This approach is suitable when the objective function and constraint violations can be described by the same measurement, for example process planning problems under demand uncertainties (Clay and Grossmann, 1997; Gupta and Maranas, 2000). This compensation, however, requires a common measurement to describe the objective function and the constraint violations.

Decision making, however, inherently involves however consideration of uncertain outcomes. Thus, one is confronted with decisions a priori for the future operation. The decision though should be made before the occurrence of the random inputs. These uncertain variables can be constant or time-dependent in the future horizon. The stochastic distribution of the uncertain variables may have different forms. The mean and variance values can be determined based on historical data analysis. However, while computational advances in mathematical programming tools have aided decision making in many areas, their greatest impact may lie in enhancing decision making under uncertainty through stochastic programming. One method of stochastic programming is the probabilistic or chance-constrained approach which focuses on the reliability of the system, i.e., the system's ability to meet feasibility in an uncertain environment. This reliability is expressed as a minimum requirement on the probability of satisfying constraints. Thus, the objective function is expressed in terms of expected value, while the constraints are expressed in terms of fractiles. In fact, stochastic optimization even with an approximated distribution is more reliable than a deterministic optimization. For the numerical optimization under probabilistic constraints, some methods have been developed and applied to several disciplines like finance and management (Prekopa, 1995; Uryasev, 2000). In chemical process operations a few applications are known to date. It has been used by, for instance, Maranas (1997) for molecular design and Petkov and Maranas (1997) for planning und scheduling of multiproduct batch plants. Additionally, several studies on model predictive control using probabilistic programming have been carried out for linear processes (Schwarm and Nikolaou, 1999). In the case of a linear relation between the uncertain input and the output constraints, an efficient approach is presented by Prekopa (1995) for stochastic variables with correlated multivariate normal distribution, where numerical integration and sampling methods are combined. For the nonlinear case, sampling techniques can generally be employed. As an alternative to efficient sampling techniques (Diwekar and Kalagnanam, 1997), in this Thesis, approaches to addressing nonlinear, steady-state as well as dynamic optimization problems under uncertainty are developed and applied to various challenging optimization tasks with uncertainties such as optimal design and operation, as well as optimal control of industrial processes under uncertainty.

Key innovations

1 Scope

The challenge in this thesis is to address large-scale, complex optimization problems under various uncertainties. To deal with the unknown operating reality a priori, optimization under both parameter uncertainty and disturbance uncertainty has to be considered. Unlike the worst case analysis, for the presented approaches the stochastic characteristics (mean, covariance, correlation) of the uncertain variables will be involved in the optimization problem. While most parameter uncertainties are usually steady-state in nature, disturbance uncertainties are dynamic and will be described as stochastic processes. 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 and internal uncertainties representing 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. However, these uncertain variables will propagate through the process to the output variables and the outputs will also be uncertain, i.e., for a nonlinear process it is very difficult to analytically describe the distribution of the outputs. To overcome this problem, chance constrained programming is proposed in this thesis to deal basically with inequality constraints, which are based on the process requirements or limitations. This implies new approaches to high-order nonlinear integration of the joint probability density function.

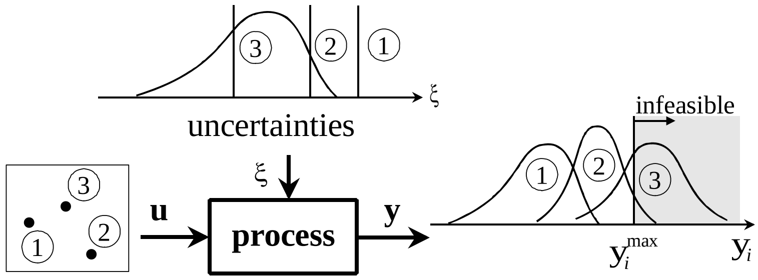

Figure 2: Strategies based on different uncertainty estimations.

Thus, the main propose is to make robust decisions accounting for uncertainties and unknown unexpected disturbances a priori. The main problem is illustrated in Figure 2. Whenever uncertainties are overestimated, the controls **u** will infer a conservative output distribution with regard to the constrained output and thus will lead to greater operational costs than actually needed (point 1 in Fig. 2). Unlike this, if the uncertainties are underestimated, the resulting strategy will be too aggressive which inevitably results in a high probability of constraint violation (point 3). Moreover, in practice, the presence of nonlinear (possibly time-varying) unmodelled dynamics and non-stationary noise or disturbances complicates the situation. How does one determine an optimal decision in such a complex setting? What is proposed in this thesis is a quantitative analysis of the probability of violating constraints by following a determined optimal strategy (point 2) based on the explicit integration of the available stochastic information of the uncertain variables. This requires a prior knowledge about the probability distribution of the output variables. Generation of this information represents one of the main contributions of this thesis.

In summary, a novel analysis and optimization framework is proposed for optimization problems under uncertainty. Based on the method of chance constrained programming, efficient solution approaches are developed to different process systems engineering problems in order to make optimal decisions by taking both performance (through the objective function) and reliability into account. The essential challenge in solving such problems lies in the computation of the probabilities of holding the constraints as well as their gradients. Due to the fact that a desired compromise between optimality and the reliability of complying with the constraints can be induced, as a result, the derived strategy is thereby neither conservative nor aggressive.

2 Overview of the Thesis

This thesis is devoted to the development of suitable algorithms and numerical techniques for the efficient solution of process engineering problems involving uncertainties. The proposed chance-constrained optimization framework forms the basis for addressing design, operation and control problems under uncertainty. The rest of the thesis is structured in seven additional Chapters. The problem formulation in **Chapter 2** reveals the necessity to explicitly incorporate the uncertainties into the optimization problems and underlines the importance of the chance constrained framework developed in this thesis. Moreover, the sources and characteristics of uncertainty and their analysis are highlighted. **Chapter 3** reviews the main approaches which have been proposed for optimization under uncertainty. **Chapter 4** describes the main principles and properties of chance constrained programming problems focusing on linear and steady-state processes. In **Chapter 5**, the new framework for chance-constrained programming of large-scale nonlinear dynamic systems under time-dependent uncertainty is introduced. The stochastic nature of the uncertainties is explicitly included in the optimization problem formulation. The method is based on the analysis of the relationship between the output constraints and the uncertain variables. The new approach involves efficient algorithms for an indirect computation of the output probability distribution so that the probabilities and their gradients can be obtained by numerical integration of the probability density function of the multivariate uncertain variables by collocation in finite elements. Furthermore, depending on the process characteristics (linear, nonlinear, steady state, dynamic), the uncertainty type (constant, time-dependent) and the form of the chance constraints (single, joint), there are 16 different possible formulations of chance-constrained problems, as illustrated in Figure 3, which can in principle be solved using the proposed framework in this thesis.

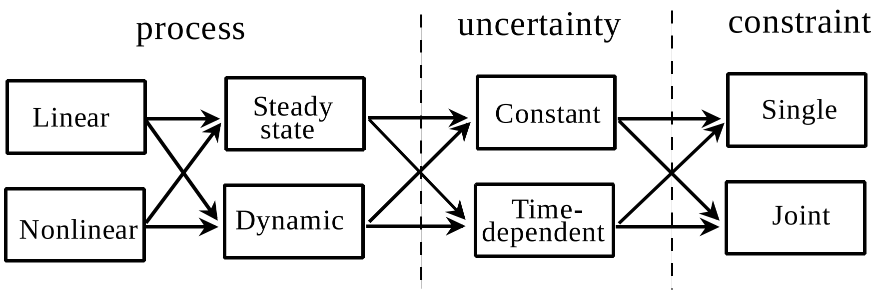

Figure 3: Classification of chance constrained problems

In order to demonstrate the efficiency of the developed approaches, in **Chapter 6** the chance-constrained optimization framework is applied to an industrial scale process, namely a reactive semi-batch distillation process. The comparison of the stochastic results with the deterministic results is presented to indicate the robustness of the stochastic optimization. These achievements are an important step towards the implementation of robust optimal operating policies on real uncertain processes.

In **Chapter 7** two methods based on a Nonlinear Model Predictive Control (NMPC) scheme are introduced to solve closed-loop dynamic optimization problems within an online framework. The key idea lies in the consideration of unknown and unexpected disturbances in advance i.e. anticipating, in particular, violation of output hard-constraints. Here, the solution of the posed novel chance-constrained NMPC problem has the features of prediction, robustness and being closed-loop. Based on the moving horizon strategy, the developed control strategy is extended to on-line optimization under uncertainty. In addition, towards an integration of dynamic real-time optimization and control of transient processes, a two-level strategy is considered.

Additionally, in all chance-constrained optimization problems under uncertainty treated in this thesis, the formulation of individual pre-defined probability limits of complying with the restrictions incorporates the issue of feasibility and the evaluation of trade-off between profitability and reliability.

Finally, a summary of the most important conclusions and key contributions are presented in **Chapter 8**. Furthermore, some suggestions and an outlook of potentially interesting future developments are presented.

3 Summary of contributions

This work presents a novel contribution to the research of optimization under uncertainty and provides theoretical developments and practical applications of chance-constrained programming. One of the main contributions is also that the solution of such problems based on the developed approaches can offer both optimal and reliable decisions such that the analysis of the outcomes allows for identifying the critical constraint which cuts off the largest part of the feasible region. This information is important for decision makers in order to relax the constraint, if necessary, so as to arrive at a meaningful decision. It has been demonstrated that probabilistic programming is a promising technique in solving optimization problems under uncertainty in process system engineering. Summarizing, the major contributions of the thesis are:

Nonlinearity between constrained output and uncertain input

The approach considers a nonlinear relation between the uncertain input and the constrained output variables. In fact, the approach is relevant to all cases when uncertainty can be described by any kind of joint correlated multivariate distribution function. The essential achievement is the efficient computation of the probabilities of holding the constraints, as well as their gradients.

Mapping back or reverse projection of output probability distribution

In systems where the relation between uncertain and constrained variables is ***nonlinear***, the type of the probability distribution function of the uncertain input is not the same as the one of the constrained output. Thus, due to the nonlinear propagation, it is difficult to obtain the stochastic distribution of output variables. For this reason, nonlinear chance-constrained programming remained an unresolved problem. In this thesis, new approaches are introduced to infer the output probability distribution. The basic idea is to avoid directly computing the output probability distribution. Instead, an equivalent representation of the probability is derived by mapping the probabilistic constrained output region back to a bounded region of the uncertain inputs. Thus, within the developed framework the probability computation of the output constraints is transformed to a multivariate integration in the limited area of uncertain inputs. Hence, the output probabilities and, simultaneously, their gradients can be calculated through multivariate integration of the density function of the uncertain inputs. For this purpose, efficient algorithms are introduced based on the orthogonal collocation on finite elements with an optimal number of collocation points. However, since multiple time intervals are considered, the reverse projection of the feasible output region is not trivial. Therefore, the approach also involves efficient algorithms for the computation of the required (mapping) reverse projection so as to deal with large-scale nonlinear dynamic processes.

Strict monotonic and non-monotonic relationship

Depending on the relation between the uncertain input and the output variables, the developed method relies upon the case of a strict monotonic relationship between the constrained output variables and at least one of the uncertain input variables. However, the chance-constrained programming framework has also been extended to address stochastic optimization problems where *no monotonic* relationship between constrained output and any uncertain input variable can be assured. Especially for those process systems where the decision variables are strongly critical to the question of whether there is monotony or not such that chance-constrained nonlinear dynamic optimization can now also be realized efficiently even for those cases where the monotony can not be guaranteed.

Consideration of single and joint constraints

In this Thesis, the focus was also on the analysis of the impact of chance constraint probability limits on the optimal policies in terms of robustness and feasibility, particularly with regard to the optimized value of the objective function. These probability limits can be seen as measurements of the robustness of the optimized strategies. Obviously a high confidence level to ensure the constraints will be preferred. However, due to the nature of the uncertain inputs and the restriction of the controls and outputs, it is often impossible to find an operation policy with a 100% guarantee for complying with the constraints. Thus a maximum confidence level needs to be found first. As part of this work, therefore, a systematic analysis, appropriate to the system complexity, has been developed to compute this value. The novelty lies in the efficient computation of single and joint constraints and their gradients.

Time-dependent uncertainties

Uncertain variables can be constant or time-dependent in the future horizon. They are, however, undetermined before their realization. Moreover, usually only a subset of variables can be measured. However, in this work novel efficient algorithms have been integrated to consider time-dependent uncertainties.

Integration of D-RTO and control level

Furthermore, for the integration of dynamic real-time optimization and control of transient processes, a two-stage strategy is considered which is characterized by an upper stage corresponding to a dynamic optimization problem and a lower stage related to a tracking control problem. For this purpose, two methods based on a nonlinear model predictive control (NMPC) scheme are proposed to solve close-loop stochastic dynamic optimization problems assuring both robustness and feasibility with respect to state output constraints within an online framework.

Dynamic adaptive back-off strategy

Feasibility and robustness with respect to input and output constraints have been achieved by the proposed backing-off strategy. The resulting NMPC scheme embedded in the on-line re-optimization framework is viable for the optimization of transient processes while simultaneously guaranteeing the constraints compliance - both for nominal operation as well as for cases of large disturbances e.g. failure situation.

Robust Nonlinear MPC under Chance Constraints

Since the prediction of future process outputs within an NMPC moving horizon is based on a process model involving the effects of manipulated inputs and disturbances on process outputs, the compliance with constraints on process outputs is more challenging than these on process inputs. Furthermore, as the model involves uncertainty, process output predictions are also uncertain. This leads to output constraints violation by the close-loop system, even though predicted outputs over the moving horizon might have been properly constrained. Thus, a robust predictive control strategy is introduced for the online optimization of transient processes, in particular, under hard constraints leading to a chance-constrained nonlinear MPC scheme where the output constraints are to be held with a predefined probability with respect to the entire horizon. Due to the moving horizon approach, the control strategy can be extended to on-line optimization under uncertainty.

Finally, a number of example problems such as batch reactors, reactor-separator system, batch distillation columns, reactor network system are discussed including the application of the optimization framework to a large-scale industrial process, namely a reactive batch distillation. Thus, the developed chance-constrained optimization framework demonstrates to be promising to address optimization problems under uncertainties. The different solution strategies have mainly been applied to transient processes. The solution provides a robust operation strategy in the future time horizon. Moreover, the relationship between the probability levels and the corresponding values of the objective function can be used for a suitable trade-off decision between profitability and robustness. Tuning the value of the different confidence levels is also an issue of the relation between feasibility and profitability.

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