Flexibility Analysis and Design Using a Parametric Programming Framework

Vikrant Bansal, John D. Perkins, and Efstratios N. Pistikopoulos
Centre for Process Systems Engineering, Dept. of Chemical Engineering, Imperial College, London SW7 2BY, U.K.

This article presents a new framework, based on parametric programming, that unifies the solution of the various flexibility analysis and design optimization problems that arise for linear, convex, and nonconvex, nonlinear systems with deterministic or stochastic uncertainties. This approach generalizes earlier work by Bansal et al. It allows (1) explicit information to be obtained on the dependence of the flexibility characteristics of a nonlinear system on the values of the uncertain parameters and design variables; (2) the critical uncertain parameter points to be identified a priori so that design optimization problems that do not require iteration between a design step and a flexibility analysis step can be solved; and (3) the nonlinearity to be removed from the optimization subproblems that need to be solved when evaluating the flexibility of systems with stochastic uncertainties.

Introduction

All chemical plants are subject to uncertainties and variations during their design and operation. Given this fact, it is clearly important for an engineer to be able to quantify the ability of a system to be operated feasibly in the presence of uncertainties (that is, conduct flexibility analysis) and to have systematic methods for designing systems that are both economically optimal and flexible. The past two decades have seen considerable advances in the development of such methods, both for deterministic cases, where the uncertain parameters are described through sets of lower and upper bounds on their values, and stochastic cases, where the uncertain parameters are described through probability distributions (for a review, see Bansal, 2000; also Table 1 summarizes the key contributions). Bansal et al. (2000) recently proposed a new approach for the flexibility analysis and design of linear systems, based on parametric programming. One of the key advantages of this approach is that it provides explicit information about the dependence of a system's flexibility on the values of the design variables. The purpose of this article is to generalize and unify this parametric programming approach for the flexibility analysis and design of nonlinear systems. The proposed framework is the first to allow a unified solution approach to be used for the various flexibility analysis and design optimization problems that arise for different types of process model and uncertainty model.

The remainder of this article is organized as follows. In the next section, various flexibility analysis and design problems are defined that have been researched in the literature. Subsequent to this, new algorithms, based on parametric programming, are presented for the solution of convex, nonlinear process models. In all cases, both mathematical and engineering examples are used to illustrate important features. Based on these developments, a conceptual framework is described that unifies the solution of the different flexibility analysis and design problems in linear, convex, and nonconvex, nonlinear systems.

Preliminary Definitions

The process model of a steady-state system can be represented by

$$h_m(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) = 0, \quad m \in M \tag{1}$$

$$g_l(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) \le 0, \quad l \in L \tag{2}$$

Correspondence concerning this article should be addressed to E. N. Pistikopoulos.
Current address of V. Bansal: Orbis Investment Advisory Limited, Orbis House, 5 Mansfield Street, London W1G 9NG, U.K.

Table 1. Literature on Flexibility Analysis and Design

Authors	Key Features
Grossmann and Morari (1983)	Review of flexibility analysis and design problems
Halemane and Grossmann (1983)	Feasibility test; design for fixed degree of flexibility
Ostrovsky et al. (1994, 1997, 2000)	Bounding algorithms for the problems considered by Halemane and Grossmann (1983)
Swaney and Grossmann (1985a,b)	Flexibility index; vertex enumeration algorithms
Kabatek and Swaney (1992)	Improved implicit vertex enumeration algorithm
Chacon-Mondragon and Himmelblau (1988, 1996)	Alternative metrics to those of Grossmann et al.; based on the proportion of feasible controls
Ierapetritou (2001)	Alternative metric based on the volume of the convex hull within the feasible operating region
Grossmann and Floudas (1987)	Active constraint strategy; MINLP formulations for feasibility test and flexibility index problems
Floudas et al. (1999)	Global optimization for the formulations of Grossmann and Floudas (1987)
Raspanti et al. (2000)	Smoothing of the MINLPs of Grossmann and Floudas (1987) using constraint aggregation
Pistikopoulos and Grossmann (1988a,b)	Retrofit design for linear systems; analytical expressions for flexibility index
Pistikopoulos and Grossmann (1989a,b)	Extension to special classes of nonlinear systems
Varvarezos et al. (1995)	Flexibility index and retrofit design for linear systems using sensitivity analysis
Pistikopoulos and Mazzuchi (1990)	Stochastic flexibility of linear systems with normally distributed parameters
Straub and Grossmann (1990)	Stochastic flexibility of linear systems with generally distributed parameters
Straub and Grossmann (1993)	Stochastic flexibility of nonlinear systems
Pistikopoulos and Ierapetritou (1995)	Design and simultaneous evaluation of stochastic flexibility of nonlinear systems
Bansal et al. (2000)	Parametric programming framework for feasibility test, flexibility index, design optimization, and stochastic flexibility of linear systems

where Eq. 1 represents the model equations; Eq. 2 represents inequalities that must be satisfied for feasible operation; and $\boldsymbol{x}$, z, $\boldsymbol{\theta}$, $\boldsymbol{d}$ and $\boldsymbol{y}$ are vectors of state variables, adjustable control variables, uncertain parameters, continuous design variables, and integer design variables, respectively. The following flexibility analysis and design problems have been defined in the literature.

Feasibility test

Given nominal values for the uncertain parameters, $\boldsymbol{\theta}^N$, expected deviations in the positive and negative directions, $\boldsymbol{\Delta\theta}^+$ and $\boldsymbol{\Delta\theta}^-$, respectively, and a set of constraints, $\boldsymbol{r}(\boldsymbol{\theta}) \leq \boldsymbol{0}$ (which may include equations correlating the uncertain parameters if they are not independent), the feasibility test problem is to determine whether, for a given design, there is at least one set of controls that can be chosen during plant operation such that, for every possible realization of the uncertain parameters, all of the constraints (Eq. 2) are satisfied. Mathematically, this is equivalent to evaluating a feasibility test measure (Halemane and Grossmann, 1983)

$$\chi(\boldsymbol{d},\boldsymbol{y}) = \max_{\boldsymbol{\theta} \in \boldsymbol{T}} \psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) \tag{3}$$

where

$$\boldsymbol{T} = \left\{ \boldsymbol{\theta} | \boldsymbol{\theta}^N - \boldsymbol{\Delta\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \boldsymbol{\Delta\theta}^+, \, \boldsymbol{r}(\boldsymbol{\theta}) \leq \boldsymbol{0} \right\} \tag{4}$$

and $\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$ is called the feasibility function, corresponding to

$$\begin{aligned} \psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) = & \min_{\boldsymbol{x},z,\boldsymbol{u}} u \\ \text{s.t.} \quad & h_m(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) = 0, \quad m \in M \\ & g_l(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) \leq u, \quad l \in L \end{aligned} \tag{5}$$

in which u is a scalar variable.

If $\chi(\boldsymbol{d},\boldsymbol{y}) \leq 0$, then a feasible operation can be ensured for all $\boldsymbol{\theta} \in \boldsymbol{T}$.

Flexibility index

The *flexibility index*, defined by (Swaney and Grossmann, 1985a), corresponds to the largest scaled deviation, δ, of any of the expected uncertain parameter deviations, $\boldsymbol{\Delta\theta}^+$ and $\boldsymbol{\Delta\theta}^-$, that a design can handle for a feasible operation. Mathematically, this is formulated as

$$\begin{aligned} & F(\boldsymbol{d},\boldsymbol{y}) = \max \delta, \\ & \text{s.t.} \quad 0 \geq \max_{\boldsymbol{\theta} \in \boldsymbol{T}(\delta)} \psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) \\ & \quad \boldsymbol{T}(\delta) = \left\{ \boldsymbol{\theta} | \boldsymbol{\theta}^N - \delta\boldsymbol{\Delta\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta\boldsymbol{\Delta\theta}^+, \, \boldsymbol{r}(\boldsymbol{\theta}) \leq \boldsymbol{0} \right\} \\ & \quad \delta \geq 0 \end{aligned} \tag{6}$$

A value of $F=1$ indicates that the design has the flexibility that exactly satisfies the most restrictive constraints on the system [in this case, a feasibility test would give $\chi(\boldsymbol{d},\boldsymbol{y})=0$].

Optimal design with fixed degree of flexibility

The objective in this problem is to find the economically optimal design that can also be operated feasibly over the set of uncertain parameters, $\boldsymbol{T}$, defined in Eq. 4 (equivalent to a flexibility index, $F=1$). Halemane and Grossmann (1983) posed this problem as

$$\min_{\boldsymbol{d},\boldsymbol{y}} E_{\boldsymbol{\theta}\in\boldsymbol{T}}\left[\min_{z} C(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})|\boldsymbol{h}=\boldsymbol{0},\ \boldsymbol{g}\leq\boldsymbol{0}\right]$$

$$\text{s.t.}\quad \max_{\boldsymbol{\theta}\in\boldsymbol{T}}\min_{z}\max_{l\in L} g_l(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})\leq 0$$

$$h_m(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})=0 \quad m\in M \tag{7}$$

where $E_{\boldsymbol{\theta}\in\boldsymbol{T}}$ is the expected cost over the possible uncertainty realizations.

Optimal design with optimal degree of flexibility

This problem is a generalization of the design problem described in the previous section. Here, the objectives are to simultaneously minimize the cost and maximize the flexibility index, while ensuring a feasible operation over the set $\boldsymbol{T}(\delta)$ (which itself is to be determined). This can be formulated as (Grossmann and Morari, 1983)

$$\min_{\boldsymbol{d},\boldsymbol{y}} E_{\boldsymbol{\theta}\in\boldsymbol{T}(\delta)}\left[\min_{z} C(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})|\boldsymbol{h}=\boldsymbol{0},\ \boldsymbol{g}\leq\boldsymbol{0}\right]$$

$$\max_{z,\delta}\delta$$

$$\text{s.t.}\quad \max_{\boldsymbol{\theta}\in\boldsymbol{T}(\delta)}\ \min_{z}\ \max_{l\in L} g_l(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})\leq 0$$

$$h_m(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})=0,\quad m\in M \tag{8}$$

Equation 8 defines an infinite number of trade-off or paretooptimal solutions where it is not possible to improve one objective without worsening the other. When $\delta=1$, Eq. 8 is equivalent to Eq. 7.

Stochastic flexibility

For a system with continuous uncertain parameters that are described by a joint probability density function (pdf), the stochastic flexibility (SF) is the probability that a given design can be operated feasibly (Pistikopoulos and Mazzuchi, 1990; Straub and Grossmann, 1990). Mathematically, this means computing

$$SF(\boldsymbol{d},\boldsymbol{y})=Pr(\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})\leq 0) \tag{9}$$

over all possible realizations of $\boldsymbol{\theta}$. The stochastic flexibility can also be expressed as the integral of the joint pdf, $j(\boldsymbol{\theta})$, over the feasible region of operation in the space of the uncertain parameters

$$SF(\boldsymbol{d},\boldsymbol{y})=\int_{\{\boldsymbol{\theta}:\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})\leq\boldsymbol{0}\}} j(\boldsymbol{\theta})\ d\boldsymbol{\theta} \tag{10}$$

Expected stochastic flexibility

The combined flexibility−availability index (Pistikopoulos et al., 1990), or *expected stochastic flexibility* (ESF) (Straub and Grossmann, 1990), is defined as

$$ESF(\boldsymbol{d})=\sum_{s=S_1}^{2^{eq}} SF(\boldsymbol{d},\boldsymbol{y}^s)\cdot P(\boldsymbol{y}^s) \tag{11}$$

where s is the index set for the system states; $P(\boldsymbol{y}^s)$ is the (discrete) probability that the system is in state s; and eq is the number of pieces of equipment in the system. Each state of the system is defined by different combinations of available and unavailable equipment. Thus, if y_i^s is a binary variable that takes a value of 1 if equipment i is available, and is zero otherwise, and p_i is the probability that equipment i is available, then

$$P(\boldsymbol{y}^s)=\prod_{\{i|y_i^s=1\}} p_i \prod_{\{i|y_i^s=0\}}(1-p_i) \tag{12}$$

Feasibility Test and Flexibility Index for Convex, Nonlinear Systems

Parametric programming approach

Consider a process model of a steady-state system where the equations are linear and the inequality constraints, $\boldsymbol{g}^{\text{convex}}$, are convex functions of the states $\boldsymbol{x}$, the controls z, the uncertain parameters $\boldsymbol{\theta}$, the continuous design variables $\boldsymbol{d}$, and the integer variables, $\boldsymbol{y}$. In this case, the feasibility function problem (Eq. 5) is

$$\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})=\min_{z,u} u$$

$$\text{s.t.}\quad \boldsymbol{0}=\boldsymbol{H_x}\cdot\boldsymbol{x}+\boldsymbol{H_z}\cdot z+\boldsymbol{H_\theta}\cdot\boldsymbol{\theta}+\boldsymbol{H_d}\cdot\boldsymbol{d}+\boldsymbol{H_y}\cdot\boldsymbol{y}+\boldsymbol{h_c} \tag{13}$$

$$u\cdot\boldsymbol{e}\geq\boldsymbol{g}^{\text{convex}}(\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$$

where $\boldsymbol{H}_{\sqcup}$, $\sqcup=\boldsymbol{x},z,\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}$, are matrices of constants; $\boldsymbol{h}_c$ is a vector of constants; $\boldsymbol{e}$ is a vector whose elements are all unity; lower and upper bounds are given on $\boldsymbol{\theta}$, $\boldsymbol{d}$, and $\boldsymbol{y}$; and there may be additional convex constraints, $\boldsymbol{r}(\boldsymbol{\theta})\leq\boldsymbol{0}$, representing relationships between dependent uncertain parameters.

Assuming that the integer variables, $\boldsymbol{y}$, are relaxed, Eq. 13 corresponds to a convex, *multiparametric nonlinear program* (mp-NLP). It has been shown that in such mp-NLPs, the objective ψ is a convex function of $\boldsymbol{\theta}$, $\boldsymbol{d}$, and $\boldsymbol{y}$ (Fiacco and Kyparisis, 1986). This convexity property can be used to approximate $\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$ by linear profiles as follows. First, an outer approximation of Eq. 13 is created by linearizing the nonlinear functions, $\boldsymbol{g}^{\text{convex}}$, at an initial feasible point. The resulting multiparametric linear program (mp-LP) is then solved exactly using the algorithm of Gal and Nedoma (1972) to give a set of linear, underestimating parametric expressions for $\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$ and a corresponding set of linear inequalities defining the regions in which these solutions are optimal. Since ψ is a convex function of $\boldsymbol{\theta}$, $\boldsymbol{d}$, and $\boldsymbol{y}$ in each region of optimality, the point of maximum discrepancy between the linear approximation and the real objective will lie at one of the verticies of the region. These vertices are identified, and if the discrepancy is greated than a user-specified tolerance, ϵ, then new outer approximations are created. The procedure is repeated until all of the underestimating approximations for $\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$ are accurate to the desired level; the final underestimators are then converted into overestimators. An algorithm for the solution of convex mp-NLPs, based on that presented by Dua and Pistikopoulos (1999), is described in the Appendix.

As previously stated, the outcome of solving Eq. 13 as a convex mp-NLP is a set of linear parametric expressions for $\psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$ and a corresponding set of linear inequalities defining the regions in which these solutions are optimal. The feasibility function expressions all have a known absolute accuracy, $\bar{\epsilon}$, which is less than or equal to the initial user-specified tolerance, ϵ. Since for convex systems the critical uncertain parameter points lie in vertex directions (Swaney and Grossmann, 1985a), exactly the same techniques as those used for linear systems (see Bansal et al., 2000) can be applied to obtain linear parametric expressions for the feasibility test measure, χ (Halemane and Grossmann, 1983), and the deterministic flexibility index, F (Swaney and Grossmann, 1985a), in terms of $\boldsymbol{d}$ and $\boldsymbol{y}$.

Algorithm 1

A parametric programming-based algorithm to solve the feasibility test and flexibility index problems for a convex process system can be developed in an analogous way to that for linear systems (Bansal et al., 2000).

Step 1. Solve the feasibility function problem (Eq. 13) as a convex mp-NLP using the method described in the Appendix. This will give a set of K linear parametric solutions, ψ^k $(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$, accurate within $\bar{\epsilon}$, and corresponding regions of optimality, CR^k.

Step 2. For each of the K feasibility functions, $\psi^k(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$, obtain the critical uncertain parameter values, $\boldsymbol{\theta}^{c,k}$. Since convex models are being considered, vertex properties can be used (Swaney and Grossmann, 1985a), that is

$$\text{(a) If } \frac{\partial \psi^k}{\partial \theta_i} < 0 \Rightarrow \Delta\theta_i^{c,k} = -\Delta\theta_i^-, \quad \theta_i^{c,k} = \theta_i^N - \delta^k \Delta\theta_i^- \qquad i=1,\ldots,n_\theta \quad (14)$$

$$\text{(b) If } \frac{\partial \psi^k}{\partial \theta_i} > 0 \Rightarrow \Delta\theta_i^{c,k} = +\Delta\theta_i^+, \quad \theta_i^{c,k} = \theta_i^N + \delta^k \Delta\theta_i^+ \qquad i=1,\ldots,n_\theta \quad (15)$$

where $\Delta\theta_i^{c,k}$ is the critical deviation of the ith uncertain parameter from its nominal value θ_i^N, and δ^k is the flexibility index associated with the kth feasibility function (Pistikopoulos and Grossmann, 1988b).

Step 3.

For the feasibility test:

(a) Substitute $\boldsymbol{\theta}^{c,k}$ with $\delta^k = 1$ into the feasibility function expressions to obtain new expressions $\psi^k(\boldsymbol{\theta}^{c,k}, \boldsymbol{d},\boldsymbol{y})$, $k=1, \ldots, K$;

(b) Obtain the set of linear solutions $\chi^k(\boldsymbol{d},\boldsymbol{y})$, and the associated regions of optimality, $\overline{CR}^k$, $k=1, \ldots, K_\chi$, where $K_\chi \le K$, by comparing the functions $\psi^k(\boldsymbol{\theta}^{c,k},\boldsymbol{d},\boldsymbol{y})$, $k=1, \ldots, K$, and retaining the upper bounds, as described in Appendix B of Bansal et al. (2000);

(c) For any desired $\bar{\boldsymbol{d}}$ and $\bar{\boldsymbol{y}}$, evaluate the feasibility test measure from $\chi(\bar{\boldsymbol{d}},\bar{\boldsymbol{y}}) = \max_k \ \chi^k(\bar{\boldsymbol{d}},\bar{\boldsymbol{y}})$. If $\chi(\bar{\boldsymbol{d}},\bar{\boldsymbol{y}}) \le 0$, then the design under investigation can be feasibly operated.

For the flexibility index:

(a) Solve the linear equations, $\psi^k[\boldsymbol{\theta}^{c,k}(\delta^k), \boldsymbol{d},\boldsymbol{y}] = 0$, $k=1, \ldots, K$, to obtain a set of linear expressions for δ^k, $k=1, \ldots, K$, in terms of $\boldsymbol{d}$ and $\boldsymbol{y}$;

(b) Obtain the set of linear solutions $F^k(\boldsymbol{d},\boldsymbol{y})$, and the associated regions of optimality, $\overline{CR}^k$, $k=1, \ldots, K_F$, by comparing the functions $\delta^k(\boldsymbol{d},\boldsymbol{y})$ and the constraints $\delta^k(\boldsymbol{d},\boldsymbol{y}) \ge 0$, $k=1, \ldots, K$, and retaining the lower bounds, as described in Appendix B of Bansal et al. (2000);

(c) For any desired $\bar{\boldsymbol{d}}$ and $\bar{\boldsymbol{y}}$, evaluate the index from $F(\bar{\boldsymbol{d}},\bar{\boldsymbol{y}}) = \min_k \ F^k(\bar{\boldsymbol{d}},\bar{\boldsymbol{y}})$.

Illustrative example

The steps of Algorithm 1 are now illustrated on a small, mathematical example. After elimination of the state variables $\boldsymbol{x}$, the system under consideration is described by the following set of reduced inequalities

$$f_1 = 0.08z^2 - \theta_1 - \frac{1}{20}\theta_2 + \frac{1}{5}d_1 - 13 \le 0$$

$$f_2 = -z - \frac{1}{3}\theta_1^{1/2} + \frac{1}{20}d_2 + 11\frac{1}{3} \le 0$$

$$f_3 = e^{0.21z} + \theta_1 + \frac{1}{20}\theta_2 - \frac{1}{5}d_1 - \frac{1}{20}d_2 - 11 \le 0 \quad (16)$$

The ranges of interest for the design variables are $10 \le d_1 \le 15$ and $2 \le d_2 \le 4$. The uncertain parameters both have nominal values of 3 and expected deviations ± 1, that is, $2 \le \theta_i \le 4$, $i=1, 2$.

Step 1. The feasibility function problem is solved as an mp-NLP, as demonstrated in detail for this example in the Appendix. Note that if the problem was solved using the ranges $2 \le \theta_i \le 4$, $i=1, 2$, then any expressions generated for the flexibility index using Algorithm 1 would only be valid in this range also, corresponding to $F \le 1$. Therefore, in order to account for designs for which the flexibility index may be greater than 1, expanded ranges of $1.5 \le \theta_i \le 4.5$, $i=1, 2$, are used. Nine parametric expressions are found, which all overestimate the real solution to within $\bar{\epsilon} = 0.0042$

$$\psi^1(\boldsymbol{\theta},\boldsymbol{d}) = 0.2052\theta_1 + 0.0150\theta_2 - 0.0601d_1 + 0.0200d_2 - 0.1983 \quad (17)$$

$$CR^1 = \begin{cases} 1.1385e3\theta_1 - \theta_2 + 4d_1 + 2d_2 \leq 2.2787e3 \\ 47.6922\theta_1 - \theta_2 - 4d_1 - 2d_2 \geq 48.3653 \\ -15.4564\theta_1 - \theta_2 + 4d_1 + 2d_2 \leq 29.9632 \end{cases}$$

$$\psi^2(\boldsymbol{\theta},\boldsymbol{d}) = 0.3011\theta_1 + 0.0176\theta_2 - 0.0704d_1 + 0.0148d_2 - 0.3661 \quad (18)$$

$$CR^2 = \{21.5714\theta_1 + \theta_2 - 4d_1 - 2d_2 \geq 45.1858$$

$$\psi^3(\boldsymbol{\theta},\boldsymbol{d}) = -0.4366\theta_1 - 0.0174\theta_2 + 0.0696d_1 + 0.0326d_2 - 1.0807 \quad (19)$$

$$CR^3 = \{-19.88899\theta_1 + \theta_2 + 4d_1 + 0.3570d_2 \leq 27.1686$$

$$\psi^4(\boldsymbol{\theta},\boldsymbol{d}) = 0.2542\theta_1 + 0.0157\theta_2 - 0.0630d_1 + 0.0185d_2 - 0.2749 \quad (20)$$

$$CR^4 = \begin{cases} 36.6166\theta_1 + \theta_2 - 4d_1 - 2d_2 \geq 44.3804 \\ 29.7325\theta_1 - \theta_2 - 4d_1 - 2d_2 \geq 53.7990 \\ 1.0561e3\theta_1 + \theta_2 - 4d_1 - 2d_2 \geq 2.9549e3 \\ 16.2974\theta_1 - \theta_2 - 4d_1 - 2d_2 \geq 1.5220 \end{cases}$$

$$\psi^5(\boldsymbol{\theta},\boldsymbol{d}) = 0.2269\theta_1 + 0.0150\theta_2 - 0.0600d_1 + 0.0200d_2 - 0.2418 \quad (21)$$

$$CR^5 = \begin{cases} 1.1385e3\theta_1 - \theta_2 + 4d_1 + 2d_2 \geq 2.2787e3 \\ 36.6166\theta_1 + \theta_2 - 4d_1 - 2d_2 \leq 44.3804 \\ -16.7554\theta_1 + \theta_2 + 4d_1 + 2d_2 \leq 12.3243 \\ 50.1890\theta_1 + \theta_2 - 4d_1 - 2d_2 \geq 37.7185 \end{cases}$$

$$\psi^6(\boldsymbol{\theta},\boldsymbol{d}) = 0.2792\theta_1 + 0.0166\theta_2 - 0.0664d_1 + 0.0168d_2 - 0.3203 \quad (22)$$

$$CR^6 = \begin{cases} 21.5714\theta_1 + \theta_2 - 4d_1 - 2d_2 \leq 45.1858 \\ 29.7325\theta_1 - \theta_2 - 4d_1 - 2d_2 \leq 53.7990 \\ 82.9110\theta_1 + \theta_2 - 4d_1 - 2d_2 \geq 260.7200 \end{cases}$$

$$\psi^7(\boldsymbol{\theta},\boldsymbol{d}) = 0.2391\theta_1 + 0.0157\theta_2 - 0.0629d_1 + 0.0185d_2 - 0.2328 \quad (23)$$

$$CR^7 = \begin{cases} 47.6922\theta_1 - \theta_2 - 4d_1 - 2d_2 \leq 48.3653 \\ 1.0561e3\theta_1 + \theta_2 - 4d_1 - 2d_2 \leq 2.9549e3 \\ -16.7554\theta_1 + \theta_2 + 4d_1 + 2d_2 \geq 12.3243 \\ 37.8790\theta_1 - \theta_2 - 4d_1 - 2d_2 \geq 62.8240 \end{cases}$$

$$\psi^8(\boldsymbol{\theta},\boldsymbol{d}) = 0.1951\theta_1 + 0.0144\theta_2 - 0.0575d_1 + 0.0213d_2 - 0.2179 \quad (24)$$

$$CR^8 = \begin{cases} -15.4564\theta_1 - \theta_2 + 4d_1 + 2d_2 \geq 29.9632 \\ -19.8899\theta_1 + \theta_2 + 4d_1 + 0.3570d_2 \geq 27.1686 \\ 50.1890\theta_1 + \theta_2 - 4d_1 - 2d_2 \leq 37.7185 \end{cases}$$

$$\psi^9(\boldsymbol{\theta},\boldsymbol{d}) = 0.2652\theta_1 + 0.0164\theta_2 - 0.0657d_1 + 0.0172d_2 - 0.2760 \quad (25)$$

$$CR^9 = \begin{cases} 16.2974\theta_1 - \theta_2 - 4d_1 - 2d_2 \leq 1.5220 \\ 82.9110\theta_1 + \theta_2 - 4d_1 - 2d_2 \leq 260.7200 \\ 37.8790\theta_1 - \theta_2 - 4d_1 - 2d_2 \leq 62.8240 \end{cases}$$

Step 2

$$\frac{\partial\psi^k}{\partial\theta_i} > 0 \Rightarrow \Delta\theta_1^{c,k} = +1, \quad \theta_i^{c,k} = 3 + \delta^k, \quad i = 1, 2, \quad k \neq 3$$

$$\frac{\partial\psi^k}{\partial\theta_i} < 0 \Rightarrow \Delta\theta_1^{c,k} = -1, \quad \theta_i^{c,k} = 3 - \delta^k, \quad i = 1, 2, \quad k = 3$$

Step 3

For the feasibility test, the critical values for both uncertain parameters are $+4$ except for ψ^3, where the critical values are both -4. After the substitution of these critical points into Eqs. 17 to 25 and the comparison of the resulting solutions, two linear expressions are obtained, corresponding to ψ^2 and ψ^6

$$\chi^1(\boldsymbol{d}) = -0.0704d_1 + 0.0148d_2 + 0.9088 \quad (26)$$

$$\overline{CR}^1 = \begin{cases} 2d_1 + d_2 \leq 22.5498 \\ d_1 \geq 10, \quad d_2 \geq 2 \end{cases}$$

$$\chi^2(\boldsymbol{d}) = -0.0664d_1 + 0.0168d_2 + 0.8631 \quad (27)$$

$$\overline{CR}^2 = \begin{cases} 2d_1 + d_2 \geq 22.5498 \\ 10 \leq d_1 \leq 15, \quad 2 \leq d_2 \leq 4 \end{cases}$$

For the feasibility index, after the solution of the linear equations $\psi^k[\boldsymbol{\theta}^{c,k}(\delta^k),\boldsymbol{d}] = 0$, and a comparison of the resulting expressions for $\delta^k(\boldsymbol{d})$, $k = 1, \ldots, 9$, two parameteric solutions are obtained, corresponding to $\psi^6 = 0$ and $\psi^9 = 0$

$$F^1(\boldsymbol{d}) = 0.2243d_1 - 0.0569d_2 - 1.9174 \quad (28)$$

$$\overline{CR}^1 = \begin{cases} 2.1883d_1 - d_2 \geq 25.0850 \\ d_1 \leq 15, \quad 2 \leq d_2 \leq 4 \end{cases}$$

$$F^2(\boldsymbol{d}) = 0.2332d_1 - 0.0610d_2 - 2.0199 \quad (29)$$

$$\overline{CR}^2 = \begin{cases} 2.1883d_1 - d_2 \leq 25.0850 \\ d_1 \geq 10, \quad 2 \leq d_2 \leq 4 \end{cases}$$

The parametric feasibility test solutions, Eqs. 26 and 27, are illustrated graphically in $\boldsymbol{d}$-space in Figure 1, while the flexibility index solutions, Eqs. 28 and 29, are shown in Figure 2.

Remarks on Algorithm 1

(1) Algorithm 1 is the first approach where for a convex, nonlinear system, the critical parameter values can be identified *a priori*, and explicit information is obtained on the dependence of the feasibility test measure and the flexibility index on the design and structural variables. As with linear systems, this latter feature gives a designer insight into which variables most strongly limit the flexibility, and reduces the evaluation of the flexibility metrics for a particular design and structure to simple function evaluations.

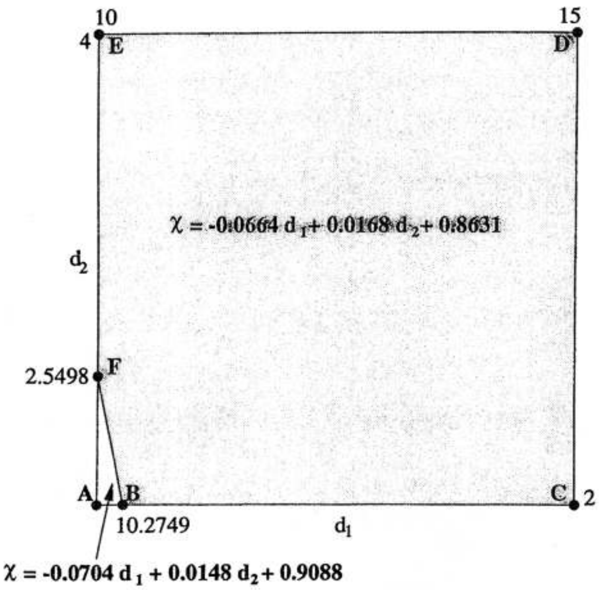

Figure 1. Parametric feasibility test solutions in *d*-space for the convex illustrative example.

(2) Tables 2 and 3 show the values of the feasibility-test measure and flexibility index for the illustrative example, found by substituting the design values at the different points indicated in Figures 1 and 2 in Eqs. 26 to 29. The tables also demonstrate the accuracy of these predicted values by comparing them with the actual solutions that were obtained by a repeated application of the vertex enumeration algorithms of Halemane and Grossmann (1983) and Swaney and Grossmann (1985a). It can be seen that the predicted values of χ are greater than the actual values, while the predicted values

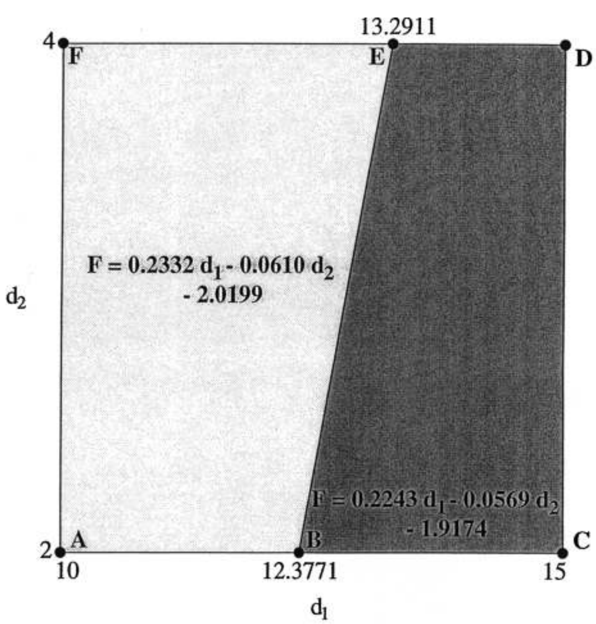

Figure 2. Parametric flexibility index solutions in *d*-space for the convex illustrative example.

Table 2. Feasibility Test for Convex Example: Predicted vs. Actual Values

Point	$\chi^{\text{predicted}}$	χ^{actual}	Error	Feasible Design?
A	0.2343	0.2336	0.0008	No
B	0.2150	0.2147	0.0003	No
C	−0.0985	−0.1012	0.0027	Yes
D	−0.0649	−0.0663	0.0015	Yes
E	0.2669	0.2653	0.0015	No
F	0.2425	0.2422	0.0003	No

of F are less than the actual values. Since the linear parametric solutions for the feasibility function ψ given by Step 1 of Algorithm 1 are always overestimators to the real solution, the feasibility test measure, defined in Eq. 3 by

$$\chi(\boldsymbol{d},\boldsymbol{y}) = \max_{\boldsymbol{\theta} \in \boldsymbol{T}} \psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) \tag{30}$$

will also always be overestimated, while the flexibility index, defined in Eq. 6 by

$$\begin{aligned} F(\boldsymbol{d},\boldsymbol{y}) &= \max\ \delta \\ \text{s.t.}\quad & 0 \geq \max_{\theta \in \boldsymbol{T}(\delta)} \psi(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y}) \\ & \boldsymbol{T}(\delta) = \left\{ \boldsymbol{\theta} | \boldsymbol{\theta}^N - \delta \boldsymbol{\Delta\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta \boldsymbol{\Delta\theta}^+,\ \boldsymbol{r}(\boldsymbol{\theta}) \leq \boldsymbol{0} \right\} \\ & \delta \geq 0 \end{aligned} \tag{31}$$

will always be underestimated. This prevents overly optimistic conclusions from being drawn about a system's flexibility characteristics.

(3) Because the exact feasibility function, ψ, is a convex function of $\boldsymbol{\theta}$, $\boldsymbol{d}$, and $\boldsymbol{y}$, from Eq. 30, χ is also a convex function of $\boldsymbol{d}$ and $\boldsymbol{y}$. This means that the point of maximum discrepancy between the linear parametric solutions given by Algorithm 1 and the actual solution lies at one of the vertices of the parametric regions of optimality (Dua and Pistikopoulos, 1999). Thus, for the illustrative example, Figure 1 and Table 2 indicate that the magnitude of the error is no greater than 0.0027 in the whole of $\boldsymbol{d}$-space, which is less than the maximum error, $\bar{\epsilon} = 0.0042$, of the feasibility function expressions (Eqs. 17–25). It should be noted, however, that if the gradient of ψ with respect to any of the uncertain parameters is of a magnitude close to zero, then the approximating linear parametric expressions for ψ generated in Step 1 of Algorithm 1 may have coefficients of $\boldsymbol{\theta}$ that are of the wrong sign. The subsequent identification of the critical uncertain

Table 3. Flexibility Index for Convex Example: Predicted vs. Actual Values

Point	$F^{\text{predicted}}$	F^{actual}	Error
A	0.1904	0.2052	0.0148
B	0.7448	0.7529	0.0081
C	1.3330	1.3468	0.0138
D	1.2193	1.2312	0.0119
E	0.8360	0.8423	0.0065
F	0.0685	0.0803	0.0119

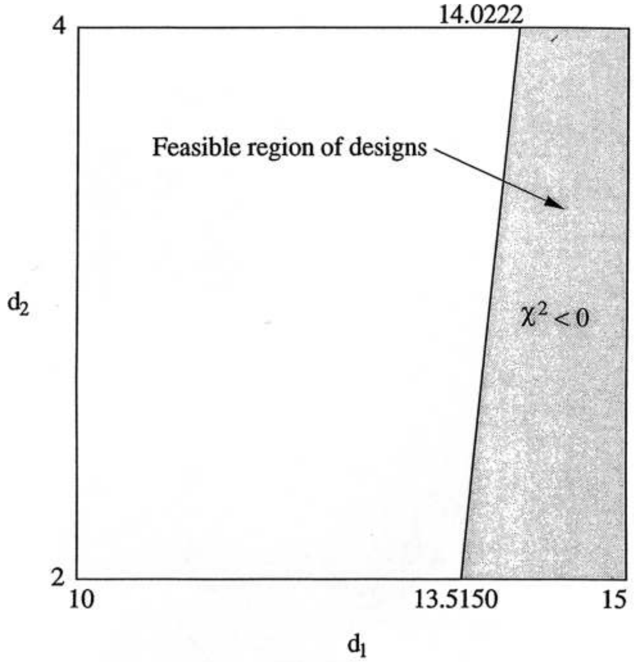

Figure 3. Feasible region in *d*-space for the convex illustrative example.

parameter values can then lead to a maximum error in χ that is slightly greater than that for ψ. In the case of the flexibility index, which from Eq. 31 is a nonconvex function of $\boldsymbol{d}$ and $\boldsymbol{y}$, the magnitude of the error will additionally depend on the expected deviations, $\boldsymbol{\Delta\theta}^-$ and $\boldsymbol{\Delta\theta}^+$, of the uncertain parameters from their nominal values.

(4) As for the linear systems, the parametric information given by Algorithm 1 for a convex, nonlinear system, allows the construction of a "feasible region" in the design space for a given structure $\bar{\boldsymbol{y}}$, through the expressions $\chi^k(\boldsymbol{d},\bar{\boldsymbol{y}}) \le 0$, $k = 1, \ldots, K_\chi$ (or, for a target flexibility index, F^t, through $F^k(\boldsymbol{d},\bar{\boldsymbol{y}}) \ge F^t$, $k = 1, \ldots, K_F$). This enables a designer to know *a priori* for which structures and ranges of design variables a convex system can be operated feasibly in the presence of uncertainties. The shaded area in Figure 3 indicates this region for the illustrative example.

(5) Although Algorithm 1 has been developed for systems of the form in Eq. 13, with the linear equalities and convex inequalities, it is also applicable for systems with nonlinear equalities that can be relaxed as convex inequalities (Acevedo and Pistikopoulos, 1996; Papalexandri and Dimkou, 1998), and for nonconvex systems where elimination of the states $\boldsymbol{x}$ leads to convexification.

(6) In principle there is no limitation on the number of uncertain parameters, design, and structural variables that the new algorithm for feasibility test and flexibility index evaluation can handle. In practice, any size limitations are due to the underlying mp-NLP algorithm employed. At present, using the method described in the Appendix, the solution of convex mp-NLPs can become unwieldy with more than about 10 parameters. Ongoing research is aimed at improving the efficiency of such mp-NLP algorithms.

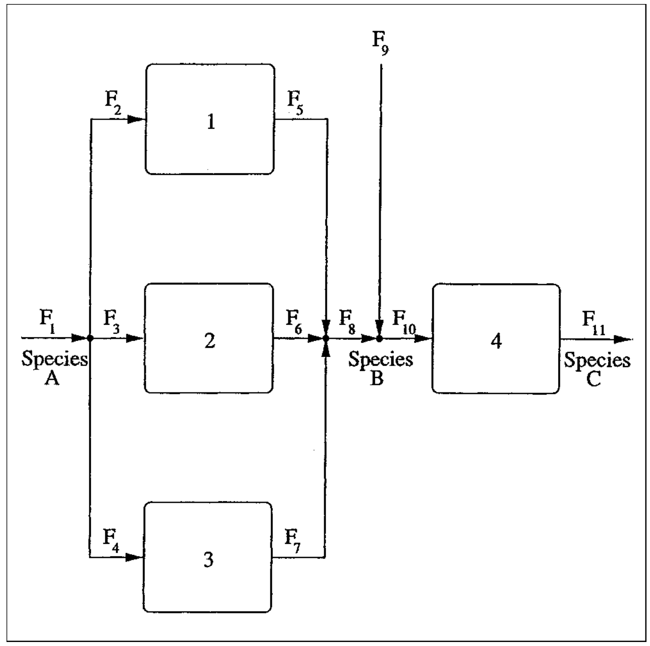

Figure 4. Process Example 1: a chemical complex.

Process Example 1

The use of Algorithm 1 is now further demonstrated on a process problem studied in various forms by Kocis and Grossmann (1987), Acevedi and Pistikopoulos (1996), Hené et al. (2002), and Bernardo et al. (1999). Figure 4 shows a system where three plants, 1, 2, and 3, each convert a raw material A into an intermediate B. This is mixed with a limited amount of fresh B before passing through plant 4, which produces the final product C. It is assumed that the supply of raw material A, denoted by S_A, is uncertain, with a nominal value of 24 and range $20 \le S_A \le 28$. Similarly, the supply of fresh B, denoted by S_B, has a nominal value of 12 and range $10 \le S_B \le 14$, while the demand for product C, D_C, is also uncertain, with the same nominal value and range as S_A. The convex process model, which consists of molar balances and specifications, is shown in Table 4. There are seven state variables, $\boldsymbol{x} = [F_1, F_5, F_6, F_7, F_8, F_{10}, F_{11}]^T$; four control variables, $\boldsymbol{z} = [F_2, F_3, F_4, F_9]^T$; three uncertain parameters, $\boldsymbol{\theta} = [S_A, S_B, D_C]^T$; and three design variables, $\boldsymbol{d} = [d_1, d_2, d_3]^T$, which correspond to the processing capacities of plants 1, 2, and 3. The ranges of interest for the latter are $8 \le d_{i(i=1,2,3)} \le 12$.

Step 1 of Algorithm 1 gives seven feasibility function expressions, which all overestimate the real solution to within

Table 4. Model for Process Example 1

Equalities	Inequalities
$h_1 = F_1 - F_2 - F_3 - F_4 = 0$	$g_1 = F_1 - S_A \le 0$
$h_2 = F_5 - 18 \ln[1 + (F_2/20)] = 0$	$g_2 = F_2 - d_1 \le 0$
$h_3 = F_6 - 20 \ln[1 + (F_3/21)] = 0$	$g_3 = F_3 - d_2 \le 0$
$h_4 = F_7 - 15 \ln[1 + (F_4/26)] = 0$	$g_4 = F_4 - d_3 \le 0$
$h_5 = F_8 - F_5 - F_6 - F_7 = 0$	$g_5 = F_9 - S_B \le 0$
$h_6 = F_{10} - F_8 - F_9 = 0$	$g_6 = D_C - F_{11} \le 0$
$h_7 = F_{11} - 0.9F_{10} = 0$	

$\bar{\epsilon} = 0.0935$:

$$\psi^1(\boldsymbol{\theta},\boldsymbol{d}) = -0.1624\theta_1 - 0.3337\theta_2 + 0.3708\theta_3 - 0.0586d_1 - 0.0744d_2 - 0.4931$$

$$CR^1 = \begin{cases} -17.2014\theta_1 - 9\theta_2 + 10\theta_3 + 12.1061d_1 + 11.7064d_2 + 12.3889d_3 \geq 24.9774 \\ -15.2549\theta_1 - 9\theta_2 + 10\theta_3 + 15.0877d_1 + 19.1673d_2 \leq 144.3570 \\ -4.0967\theta_1 - 9\theta_2 + 10\theta_3 + 13.4523d_1 + 9.6444d_2 \leq 273.9111 \\ 20.5941\theta_1 + 9\theta_2 - 10\theta_3 - 14.0535d_1 - 10.8057d_2 - 14.7349d_3 \leq 29.9539 \\ 68.2943\theta_1 + 9\theta_2 - 10\theta_3 - 44.1790d_1 - 43.1153d_2 \leq 783.4444 \\ -16.7132\theta_1 - 9\theta_2 + 10\theta_3 + 25.1263d_1 + 10.5869d_2 \leq 115.5185 \end{cases}$$

$$\psi^2(\boldsymbol{\theta},\boldsymbol{d}) = -0.2487\theta_2 + 0.2764\theta_3 - 0.1729d_1 - 0.1850d_2 - 0.1170d_3 - 0.2572$$

$$CR^2 = \begin{cases} -17.2014\theta_1 - 9\theta_2 + 10\theta_3 + 12.1061d_1 + 11.7064d_2 + 12.3889d_3 \leq 24.9774 \\ -9\theta_2 + 10\theta_3 + 2.2325d_1 + 16.2731d_2 + 0.4944d_3 \leq 303.4833 \\ -14.5843\theta_1 - 9\theta_2 + 10\theta_3 + 10.4632d_1 + 10.0975d_2 + 13.0235d_3 \leq 66.3869 \end{cases}$$

$$\psi^3(\boldsymbol{\theta},\boldsymbol{d}) = -0.2217\theta_1 - 0.3687\theta_2 + 0.4096\theta_3 - 1.0537$$

$$CR^3 = \begin{cases} -15.2549\theta_1 - 9\theta_2 + 10\theta_3 + 15.0877d_1 + 19.1673d_2 \geq 144.3570 \\ 36.8930\theta_1 + 9\theta_2 - 10\theta_3 - 18.2591d_1 - 37.6340d_2 \leq 106.8750 \\ -13.5139\theta_1 - 9\theta_2 + 10\theta_3 + 31.0257d_1 + 29.4113d_2 \geq 178.7872 \end{cases}$$

$$\psi^4(\boldsymbol{\theta},\boldsymbol{d}) = -0.1729\theta_1 - 0.3568\theta_2 + 0.3964\theta_3 - 0.0241d_1 - 0.0497d_2 - 1.1949$$

$$CR^4 = \begin{cases} -4.0967\theta_1 - 9\theta_2 + 10\theta_3 + 13.4523d_1 + 9.6444d_2 \geq 273.9111 \\ 36.8930\theta_1 + 9\theta_2 - 10\theta_3 - 18.2591d_1 - 37.6340d_2 \geq 106.8750 \\ -16.5488\theta_1 - 9\theta_2 + 10\theta_3 + 13.9061d_1 + 10.5209d_2 + 11.1218d_3 \geq 44.5559 \\ -13.8699\theta_1 - 9\theta_2 + 10\theta_3 + 18.1300d_1 + 14.7399d_2 \geq 112.9436 \\ 55.3060\theta_1 - 9\theta_2 + 10\theta_3 - 41.5127d_1 + 5.2066d_2 \geq 1019.6726. \end{cases}$$

$$\psi^5(\boldsymbol{\theta},\boldsymbol{d}) = -0.2628\theta_2 + 0.2919\theta_3 - 0.1694d_1 - 0.1597d_2 - 0.1162d_3 - 0.7293$$

$$CR^5 = \begin{cases} 20.5941\theta_1 + 9\theta_2 - 10\theta_3 - 14.0535d_1 - 10.8057d_2 - 14.7349d_3 \geq 29.9539 \\ -9\theta_2 + 10\theta_3 + 2.2325d_1 + 16.2731d_2 + 0.4944d_3 \geq 303.4833 \\ -16.5488\theta_1 - 9\theta_2 + 10\theta_3 + 13.9061d_1 + 10.5209d_2 + 11.1218d_3 \leq 44.5559 \\ -17.6390\theta_1 - 9\theta_2 + 10\theta_3 + 12.1872d_1 + 8.8040d_2 + 15.6478d_3 \leq 16.7260 \end{cases}$$

$$\psi^6(\boldsymbol{\theta},\boldsymbol{d}) = -0.1310\theta_1 - 0.3296\theta_2 + 0.3662\theta_3 - 0.0789d_1 - 0.0943d_2 - 0.8535$$

$$CR^6 = \begin{cases} 68.2943\theta_1 + 9\theta_2 - 10\theta_3 - 44.1790d_1 - 43.1153d_2 \geq 783.4444 \\ -14.5843\theta_1 - 9\theta_2 + 10\theta_3 + 10.4632d_1 + 10.0975d_2 + 13.0235d_3 \geq 66.3869 \\ -13.8699\theta_1 - 9\theta_2 + 10\theta_3 + 18.1300d_1 + 14.7399d_2 \geq 112.9436 \\ -17.6390\theta_1 - 9\theta_2 + 10\theta_3 + 12.1872d_1 + 8.8040d_2 + 15.6478d_3 \geq 16.7260 \end{cases}$$

$$\psi^7(\boldsymbol{\theta},\boldsymbol{d}) = -0.1977\theta_1 - 0.3528\theta_2 + 0.3919\theta_3 - 0.0055d_1 - 0.0521d_2 - 0.7372$$

$$CR^7 = \begin{cases} -16.7132\theta_1 - 9\theta_2 + 10\theta_3 + 25.1263d_1 + 10.5869d_2 \geq 115.5185 \\ -13.5139\theta_1 - 9\theta_2 + 10\theta_3 + 31.0257d_1 + 29.4113d_2 \leq 178.7872 \\ 55.3060\theta_1 - 9\theta_2 + 10\theta_3 - 41.5127d_1 + 5.2066d_2 \leq 1019.6726 \end{cases}$$

In all cases the critical directions for the uncertain parameters are toward the lower bounds for θ_1 and θ_2, and toward the upper bound for θ_3. One expression for the feasibility test measure is then obtained that is independent of the values of the design variables, and is valid over the whole range of $\boldsymbol{d}$

$$\chi(\boldsymbol{d}) = \psi^3(\boldsymbol{\theta}^{c,3},\boldsymbol{d}) = 2.2963$$

Table 5. Feasibility Test for Process Example 1: Predicted vs. Actual Values

d^T	$\chi^{\text{predicted}}$	χ^{actual}	Error	Feasible Design?
(8,8,8)	2.2963	2.2451	0.0512	No
(8,8,12)	2.2963	2.2451	0.0512	No
(12,8,8)	2.2963	2.2313	0.0650	No
(12,8,12)	2.2963	2.2313	0.0650	No
(8,12,8)	2.2963	2.2028	0.0935	No
(8,12,12)	2.2963	2.2028	0.0935	No
(12,12,8)	2.2963	2.2028	0.0935	No
(12,12,12)	2.2963	2.2028	0.0935	No

Since $\chi > 0$, this indicates that there are no plant capacities within the given ranges for which the system can be operated feasibly over the whole ranges of the uncertain supplies and demand, even with the manipulation of the control variables during operation. Table 5 compares the predicted value of χ with the exact values given by a vertex enumeration approach (Halemane and Grossmann, 1983) at the vertices of the design space. As discussed in remark 3 in the previous section of this article, since χ is a convex function of $\boldsymbol{d}$, the point of maximum discrepancy lies at one of these vertices. It can be seen that in this case the maximum error is the same as that for the feasibility functions, namely $\bar{\epsilon} = 0.0935$.

Four expressions are obtained from Step 3 of Algorithm 1 for the flexibility index, corresponding to $\psi^1 = 0$, $\psi^3 = 0$, $\psi^4 = 0$, and $\psi^7 = 0$. These are all independent of the processing capacity of plant 3

$$F^1(\boldsymbol{d}) = 0.0209d_1 + 0.0266d_2 - 0.1798$$

$$\overline{CR}^1 = \begin{cases} 1.2914d_1 + d_2 \leq 21.8219 \\ 1.9948d_1 + d_2 \leq 29.2749 \end{cases}$$

$$F^2(\boldsymbol{d}) = 0.2962$$

$$\overline{CR}^2 = \begin{cases} 0.4852d_1 + d_2 \geq 15.5623 \\ 0.1055d_1 + d_2 \geq 11.4899 \end{cases}$$

$$F^3(\boldsymbol{d}) = 0.0081d_1 + 0.01662d_2 + 0.0375$$

$$\overline{CR}^3 = \begin{cases} 1.2914d_1 + d_2 \geq 21.8219 \\ 0.4852d_1 + d_2 \leq 15.5623 \\ 17.1793d_1 - d_2 \leq 173.9049 \end{cases}$$

$$F^4(\boldsymbol{d}) = 0.0018d_1 + 0.0170d_2 + 0.1010$$

$$\overline{CR}^4 = \begin{cases} 1.9948d_1 + d_2 \geq 29.2749 \\ 0.1055d_1 + d_2 \leq 11.4899 \\ 17.1793d_1 - d_2 \geq 173.9049 \end{cases}$$

The preceding parametric expressions are illustrated graphically in Figure 5, while the accuracy of the predicted values at the various points indicated in the diagram is demonstrated in Table 6. For this example, the errors are all substantially less than that of the feasibility functions and feasibility test measure, $\bar{\epsilon} = 0.0935$.

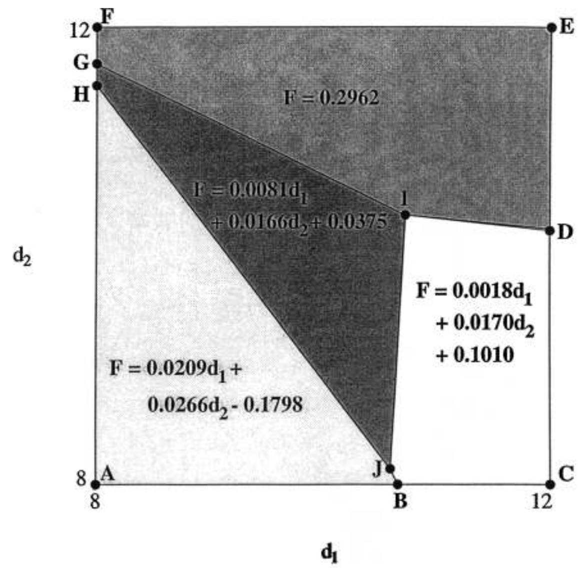

Figure 5. Parametric flexibility index solutions in $\boldsymbol{d}$-space for process Example 1.

Design Optimization of Convex, Nonlinear Systems

Existing solution approaches

The design problems defined in Eqs. 7 and 8 both correspond to optimization problems with an infinite number of search variables (since for every realization of $\boldsymbol{\theta}$ an optimal z is chosen), and as such are extremely difficult to solve exactly. Halemane and Grossmann (1983) built on previous work by Grossmann and Sargent (1978) to show that the solution of Eq. 7 can be approximated by applying the following iterative algorithm (Biegler et al., 1997).

Step 1. Choose an initial set of uncertainty scenarios $\boldsymbol{\theta}^i$, $i = 1, \ldots, ns$. This may consist, for example, of the nominal point and some vertex points.

Step 2. For the current set of scenarios, obtain a design $(\boldsymbol{d}^*, \boldsymbol{y}^*)$ by solving the multiperiod design optimization problem

$$\min_{\boldsymbol{d},\boldsymbol{y},z^1,z^2,\ldots,z^{ns}} \left\{ \sum_{i=1}^{ns} w_i \cdot C(\boldsymbol{x}^i, z^i, \boldsymbol{\theta}^i, \boldsymbol{d}, \boldsymbol{y}) \right\}$$

s.t.

$$h_m(\boldsymbol{x}^i, z^i, \boldsymbol{\theta}^i, \boldsymbol{d}, \boldsymbol{y}) = 0, \quad m \in M$$

$$g_l(\boldsymbol{x}^i, z^i, \boldsymbol{\theta}^i, \boldsymbol{d}, \boldsymbol{y}) \leq 0, \quad l \in L, \quad i = 1, \ldots, ns \qquad (32)$$

where w_i are discrete probabilities for the selected parameter points $\boldsymbol{\theta}^i$ ($\sum_{i=1}^{ns} w_i = 1$), and are usually chosen based on engineering judgement. Equation 32 corresponds to an MINLP due to the presence of the integer (usually binary) design variables $\boldsymbol{y}$.

Step 3. Test the design from Step 2 for feasibility over all the ranges of the uncertain parameters by solving Eq. 3. If $\chi(\boldsymbol{d}^*, \boldsymbol{y}^*) \leq 0$, then the system is feasible and the algorithm terminates; otherwise, the solution of Eq. 3 defines a critical point that is then added to the set of scenarios, before returning to Step 2.

Table 6. Flexibility Index for Process Example 1: Predicted vs. Actual Values

Point	(d_1, d_2)	$F^{\text{predicted}}$	F^{actual}	Error
A	(8,8)	0.2002	0.2270	0.0268
B	(10.6653,8)	0.2560	0.2718	0.0158
C	(12,8)	0.2584	0.2824	0.0240
D	(12,10.2240)	0.2962	0.3140	0.0179
E	(12,12)	0.2962	0.3241	0.0279
F	(8,12)	0.2962	0.3036	0.0074
G	(8,11.6809)	0.2962	0.3002	0.0040
H	(8,11.4903)	0.2930	0.2979	0.0049
I	(10.7259,10.3584)	0.2962	0.3124	0.0162
J	(10.5966,8.1369)	0.2582	0.2742	0.0160

The usual approach that is employed for solving Eq. 8 is to simply solve it at a number of different values of δ (Grossmann and Morari, 1983) that is, apply the preceding algorithm using different sets $\boldsymbol{T}$ in Step 3. A trade-off curve of cost vs. flexibility index can then be drawn up and the engineer can choose a design.

Parametric programming approach

Multiparametric programming can be used to avoid the iteration required between Steps 2 and 3. First, by applying Algorithm 1, all of the critical points of the uncertain parameters are identified *a priori* and analytical expressions are obtained for the feasibility test measure and the flexibility index. The problem of optimal design for a fixed degree of flexibility can then be determined by solving the convex MINLP

$$\min_{\boldsymbol{d},\boldsymbol{y},z^1,z^2,\ldots,z^{ns}} \left[\sum_{i=1}^{ns} w_i \cdot C^{\text{convex}}\left(\boldsymbol{x}^i,\boldsymbol{z}^i,\boldsymbol{\theta}^i,\boldsymbol{d},\boldsymbol{y}\right) \right]$$

s.t.

$$h_m^{\text{linear}}\left(\boldsymbol{x}^i,\boldsymbol{z}^i,\boldsymbol{\theta}^i,\boldsymbol{d},\boldsymbol{y}\right) = 0, \quad m \in M, \quad i = 1, \ldots, ns$$
$$g_l^{\text{convex}}\left(\boldsymbol{x}^i,\boldsymbol{z}^i,\boldsymbol{\theta}^i,\boldsymbol{d},\boldsymbol{y}\right) \le 0, \quad l \in L, \quad i = 1, \ldots, ns$$
$$\chi^k(\boldsymbol{d},\boldsymbol{y}) \le 0, \quad k = 1, \ldots, K_\chi \tag{33}$$

where the set $\boldsymbol{\theta}^i$, $i = 1, \ldots, ns$, consists of the critical points identified in Steps 2 and 3a of Algorithm 1 that lead to the final set of parametric expressions $\chi^k(\boldsymbol{d},\boldsymbol{y})$, $k = 1, \ldots, K_\chi$, as well as other points, such as the nominal one.

Similarly, the more general problem of optimal design with optimal degree of flexibility can be formulated as

$$\min_{\boldsymbol{d},\boldsymbol{y},z^1,z^2,\ldots,z^{ns}} \left\{ \sum_{i=1}^{ns} w_i \cdot C^{\text{convex}}\left[\boldsymbol{x}^i,\boldsymbol{z}^i,\boldsymbol{\theta}^i(F^t),\boldsymbol{d},\boldsymbol{y}\right] \right\}$$

s.t.

$$h_m^{\text{linear}}\left[\boldsymbol{x}^i,\boldsymbol{z}^i,\boldsymbol{\theta}^i(F^t),\boldsymbol{d},\boldsymbol{y}\right] = 0, \quad m \in M, \quad i = 1, \ldots, ns$$
$$g_l^{\text{convex}}\left[\boldsymbol{x}^i,\boldsymbol{z}^i,\boldsymbol{\theta}^i(F^t),\boldsymbol{d},\boldsymbol{y}\right] \le 0, \quad l \in L, \quad i = 1, \ldots, ns$$
$$F^k(\boldsymbol{d},\boldsymbol{y}) \ge F^t, \quad k = 1, \ldots, K_F \tag{34}$$

where the critical points within $\boldsymbol{\theta}^i$, $i = 1, \ldots, ns$, are functions of the target flexibility index, F^t, since they are identified in Step 3b of Algorithm 1 with $\delta^k = F^t$, $k = 1, \ldots, K$. Instead of having to solve Eq. 34 repeatedly for different values of the target flexibility index, F^t, Eq. 34 can be solved as a convex, single-parameter, mixed-integer nonlinear program (p-MINLP) in F^t to explicitly yield all the cost solutions as linear functions of F^t.

Illustrative example

In order to demonstrate the use of the parametric programming approach just proposed compared to existing solution approaches, consider the illustrative example that was used earlier in this article with an economic-objective function that depends only on $\boldsymbol{d}$. Using existing solution approaches, the first step is to pose the design optimization problem as

$$\text{Cost} = \min_{d_1,d_2} \left(\frac{d_1^2}{25} + \frac{d_2^2}{4} \right)$$

s.t.

$$f_1 = 0.08(z^i)^2 - \theta_1^i - \frac{1}{20}\theta_2^i + \frac{1}{5}d_1 - 13 \le 0, \quad i = 1, \ldots, ns$$
$$f_2 = -z^i - \frac{1}{3}\left(\theta_1^i\right)^{1/2} + \frac{1}{20}d_2 + 11\frac{1}{3} \le 0, \quad i = 1, \ldots, ns$$
$$f_3 = e^{0.21z^i} + \theta_1^i + \frac{1}{20}\theta_2^i - \frac{1}{5}d_1 - \frac{1}{20}d_2 - 11 \le 0, \quad i = 1, \ldots, ns$$
$$3 - F^t \le \theta_{1,2}^i \le 3 + F^t, \quad i = 1, \ldots, ns$$
$$10 \le d_1 \le 15$$
$$2 \le d_2 \le 4$$

The preceding convex NLP is solved with the uncertain parameters initially at their nominal values, that is, $\theta_1^1 = \theta_2^1 = 3$. For $F^t = 1$, for example, a design $d_1 = 10$, $d_2 = 2$, is obtained with a cost of 5 units. The next step is to test this design over the whole range of uncertain parameters. This could be accomplished, for example, by using the vertex formulation of Halemane and Grossmann (1983). For the preceding example, the critical vertex is $\boldsymbol{\theta} = [4,4]^T$, where $\chi = 0.2335$. This point becomes the second scenario and Eq. 35 is solved again to give a new design, $d_1 = 13.46$, $d_2 = 2$, with a cost of 8.25 units. This design is then tested and found to be feasible in the whole space of $\boldsymbol{\theta}$, so the algorithm terminates. In order to generate the trade-off curve of cost against flexibility, this involved a procedure that needs to be repeated again at numerous fixed values of F^t.

In contrast to this, using the flexibility index expressions, Eqs. 28 and 29, provided by Algorithm 1, the problem can be neatly posed in the form of Eq. 34

$$\text{Cost}\ (F^t) = \min_{d_1,d_2} \left(\frac{d_1^2}{25} + \frac{d_2^2}{4} \right)$$

s.t.

$$F^1 = 0.2243d_1 - 0.0569d_2 - 1.9174 \ge F^t$$
$$F^2 = 0.2332d_1 - 0.0610d_2 - 2.0199 \ge F^t$$
$$10 \le d_1 \le 15$$
$$2 \le d_2 \le 4 \tag{35}$$

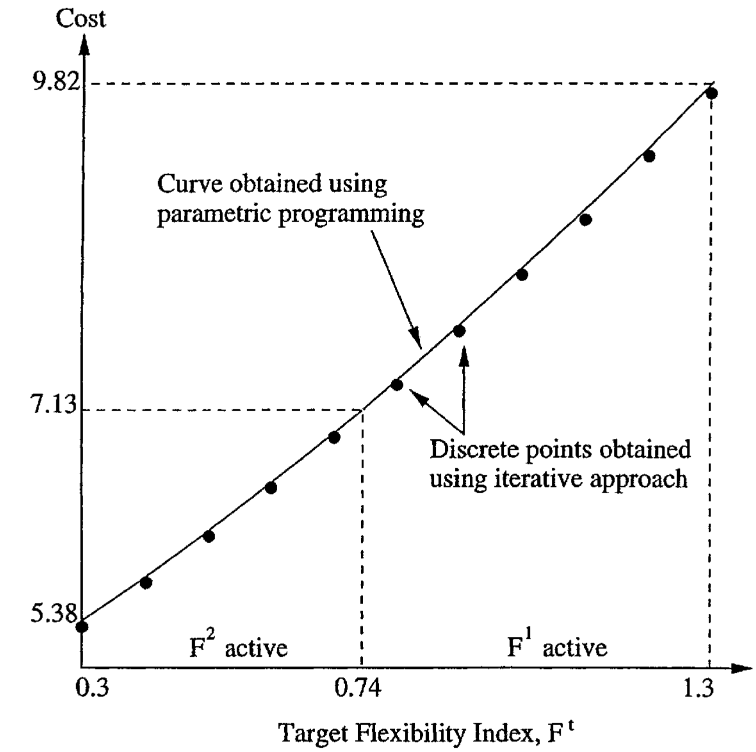

Figure 6. Cost vs. flexibility index trade-off curve for the convex illustrative example.

Equation 35 can be solved as a convex p-NLP; however, with its quadratic objective function and linear constraints, Eq. 35 actually corresponds to a parametric quadratic program (p-QP), for which specialized techniques exist to solve it exactly (for example, Berkelaar et al., 1997; Dua et al., 2002). Solving Eq. 35 as a p-QP in the range $0.3 \le F^t \le 1.3$ yields the algebraic form of the cost-flexibility trade-off curve

$$\mathrm{Cost}^1 = 0.7354(F^t)^2 + 3.1502F^t + 4.3736 \tag{36}$$

$$\overline{CR}^1 = \{0.3 \le F^t \le 0.7448$$

$$\text{Active constraint: } F^2 = F^t$$

$$\mathrm{Cost}^2 = 0.7952(F^t)^2 + 3.2304F^t + 4.2807 \tag{37}$$

$$\overline{CR}^2 = \{0.7448 \le F^t \le 1.3$$

$$\text{Active constraint: } F^1 = F^t$$

The slightly nonlinear trade-off curve defined by the parametric solutions (Eqs. 36 and 37) is shown in Figure 6, together with a number of points obtained using the nonparametric, iterative approach described earlier. It can be seen that there is very good agreement between the two sets of results.

Stochastic Flexibility of Convex, Nonlinear Systems

Algorithm 2

In an entirely analogous way to that described for linear systems in Bansal et al. (2000), a parametric programming-based algorithm for the evaluation of the stochastic flexibility of convex, nonlinear systems can be developed.

Step 1. Obtain the linear feasibility functions $\psi^k(\boldsymbol{\theta},\boldsymbol{d},\boldsymbol{y})$, $k = 1, \ldots, K$, by applying Step 1 of Algorithm 1 described earlier in the article.

Step 2. For $i = 1$ to n_θ:

(a) Compute the upper and lower bounds of θ_i in the feasible operating region, $\theta_i^{\max}$ and $\theta_i^{\min}$, respectively, as linear functions of lower-dimensional parameters, $\theta_{p(p=1,\ldots,i-1)}$, $\boldsymbol{d}$ and $\boldsymbol{y}$ (Acevedo and Pistikopoulos, 1997a), by solving the mp-LP

$$\max \left(\theta_i^{\max\, q_1\cdots q_{i-1}} - \theta_i^{\min\, q_1\cdots q_{i-1}}\right) \tag{38}$$

$$\text{s.t.} \quad \psi^k\left(\theta_{j(j=i+1,\ldots,n_\theta)}^{aq_1\cdots q_{i-1}},\ \theta_i^{\max q_1\cdots q_{i-1}},\ \theta_{p(p=1,\ldots,i-1)}^{q_1\cdots q_p},\boldsymbol{d},\boldsymbol{y}\right) \le 0, \quad k = 1, \ldots, K$$

$$\psi^k\left(\theta_{j(j=i+1,\ldots,n_\theta)}^{bq_1\cdots q_{i-1}},\ \theta_i^{\min q_1\cdots q_{i-1}},\ \theta_{p(p=1,\ldots,i-1)}^{q_1\cdots q_p},\ \boldsymbol{d},\boldsymbol{y}\right) \le 0, \quad k = 1, \ldots, K$$

$$\theta_j^L \le \theta_j^{aq_1\cdots q_{i-1}},\ \theta_j^{bq_1\cdots q_{i-1}} \le \theta_j^U,\ j = i+1, \ldots, n_\theta$$

$$\theta_i^L \le \theta_i^{\min q_1\cdots q_{i-1}} \le \theta_i^{\max q_1\cdots q_{i-1}} \le \theta_i^U$$

$$\theta_p^L \le \theta_p^{q_1\cdots q_p} \le \theta_p^U,\ p = 1, \ldots, i-1$$

$$\boldsymbol{d}^L \le \boldsymbol{d} \le \boldsymbol{d}^U$$

$$\boldsymbol{y}^L \le \boldsymbol{y} \le \boldsymbol{y}^U$$

Here, θ_j^a and θ_j^b reflect the fact that different values of θ_j, $j = i+1, \ldots, n_\theta$, must be chosen in order to calculate the upper and lower bounds on θ_i; q_i is the index set for the quadrature points to be used for the ith parameter; and $\boldsymbol{y}^L$ and $\boldsymbol{y}^U$ will usually be **0** and **1**, respectively. The solution of Eq. 38 gives N_i solutions and corresponding regions of optimality in $\theta_{p(p=1,\ldots,i-1)}$, $\boldsymbol{d}$ and $\boldsymbol{y}$.

Note that lower and upper bounds on the uncertain parameters can be obtained by truncating the probability distribution at points beyond which there is a negligible change in probability. For example, for a normally distributed parameter with mean μ and standard deviation σ, bounds of $\theta^L = \mu - 4\sigma$ and $\theta^U = \mu + 4\sigma$ can be used.

(b) Express the quadrature points, $\theta_i^{q_1 \cdots q_i}$, in terms of the locations of Gauss–Legendre quadrature points in the $[-1,1]$ interval (Carnahan et al., 1969), $\nu_i^{q_i}$, from

$$\theta_i^{q_1\cdots q_i}(\boldsymbol{d},\boldsymbol{y}) = \frac{1}{2}\left[\theta_i^{\max q_1\cdots q_{i-1}}(1+\nu_i^{q_i}) + \theta_i^{\min q_1\cdots q_{i-1}}(1-\nu_i^{q_i})\right], \quad \forall q_i \quad (39)$$

Step 3.

$$SF(\boldsymbol{d},\boldsymbol{y}) = \frac{\theta_1^{\max} - \theta_1^{\min}}{2}\sum_{q_1=1}^{Q_1} w_1^{q_1}\frac{\theta_2^{\max q_1} - \theta_2^{\min q_1}}{2}\cdots \sum_{q_{n_\theta}=1}^{Q_{n_\theta}} w_{n_\theta}^{q_{n_\theta}} j(\theta_1^{q_1}, \ldots, \theta_{n_\theta}^{q_1\cdots q_{n_\theta}}) \quad (40)$$

where $w_i^{q_i}$, $q_i = 1, \ldots, Q_i$, are the weights of the Gauss–Legendre quadrature points (Carnahan et al., 1969) for the ith parameter.

Illustrative example

Consider the problem of evaluating the stochastic flexibility of the system described by the reduced inequalities (Eq. 16), where θ_1 is uniformly distributed on the interval [2,4], and $\theta_2 \sim N$ (3, 1/16). The solution of the mp-NLP in Step 1 of Algorithm 2 gives the nine feasibility function expressions, Eqs. 17–25. In Step 2a, two mp-LPs are solved using the algorithm of Gal and Nedoma (1972), giving

$$\theta_1^{\max} = 0.2477d_1 - 0.0647d_2 + 0.9169, \quad \theta_1^{\min} = 2$$

$$CR^{1,1} = \begin{cases} 2.2443d_1 - d_2 \le 24.7992 \\ 10 \le d_1, \quad 2 \le d_2 \le 4 \end{cases}$$

$$\theta_1^{\max} = 0.2376d_1 - 0.0602d_2 + 1.0281, \quad \theta_1^{\min} = 2$$

$$CR^{1,2} = \begin{cases} 2.2443d_1 - d_2 \ge 24.7992 \\ 3.9436d_1 - d_2 \le 49.3264 \\ 2 \le d_2 \le 4 \end{cases}$$

$$\theta_1^{\max} = 4, \quad \theta_1^{\min} = 2$$

$$CR^{1,3} = \begin{cases} 3.9436d_1 - d_2 \ge 49.3264 \\ d_1 \le 15, \quad 2 \le d_2 \le 4 \end{cases}$$

$$\theta_2^{\max q_1} = 4, \quad \theta_2^{\min q_1} = 2$$

$$CR^{2,1} = \begin{cases} 16.1509\theta_1^{q_1} - 4d_1 + 1.0455d_2 \le 12.8091 \\ 16.8348\theta_1^{q_1} - 4d_1 + 1.0143d_2 \le 15.3078 \end{cases}$$

$$\theta_2^{\max q_1} = -16.1509\theta_1^{q_1} + 4d_1 - 1.0455d_2 + 16.8091$$

$$\theta_2^{\min q_1} = 2$$

$$CR^{2,2} = \begin{cases} 12.8091 \le 16.1509\theta_1^{q_1} - 4d_1 + 1.0455d_2 \le 14.8091 \\ 21.9210\theta_1^{q_1} + d_2 \le 80.0893 \end{cases}$$

$$\theta_2^{\max q_1} = -16.8348\theta_1^{q_1} + 4d_1 - 1.0143d_2 + 19.3078$$

$$\theta_2^{\min q_1} = 2$$

$$CR^{2,3} = \begin{cases} 15.3078 \le 16.8348\theta_1^{q_1} - 4d_1 + 1.0143d_2 \le 17.3078 \\ 21.9210\theta_1^{q_1} + d_2 \ge 80.0893 \end{cases}$$

The stochastic flexibility for a given set of design variables and quadrature points can be calulated by substituting the relevant values in the preceding expressions, together with Eqs. 39 and 40, where for this example the bivariate probability density function defined by θ_1 and θ_2 is given by

$$j(\theta_1^{q_1}, \theta_2^{q_1q_2}) = \sqrt{\frac{2}{\pi}}\cdot\exp\left[-8(\theta_2^{q_1q_2} - 3)^2\right]$$

Table 7 shows the stochastic flexibility results for various designs and illustrates their accuracy by comparing them with the values obtained using the sequential approach of Straub and Grossmann (1993).

Remarks on Algorithm 2

(1) Algorithm 2 provides the explicit dependence of the uncertain parameter bounds, and ultimately the stochastic flexibility of convex, nonlinear system, on the values of the design variables, and the parameters of the quadrature method being used. By applying the algorithm once, the stochastic flexibility can be evaluated for a given design and structure, for any number of quadrature points, by performing a series of function evaluations. This is demonstrated in Table 7 where no further optimization subproblems need to be solved in order to obtain the stochastic flexibilities of the second to fifth designs.

(2) Algorithm 2 leads to a significant reduction in the number of optimization subproblems that need to be solved compared with existing approaches for stochastic flexibility evaluation. If the same number of quadrature points, Q, is used for each uncertain parameter, the sequential approaches of Straub and Grossmann (1993) and Pistikopoulos and Ierapetritou (1995) require the solution of $\sum_{i=1}^{n_\theta} Q^{i-1}$ NLPs. Algorithm 2, on the other hand, only requires the solution of one mp-NLP and n_θ mp-LPs. The potential benefit of this for the illustrative example can be seen in Table 7. Generating the stochastic flexibilities shown requires the solution of a total of 490 NLPs using the sequential approach compared to just 1, albeit more difficult to solve, mp-NLP and 2 mp-LPs with Algorithm 2. Thus, we would expect the parametric programming approach to be beneficial for prob-

Table 7. SF of Convex Illustrative Example: Parametric vs. Sequential Approach

d^T	$Q_1 = Q_2$	Stochastic Flexibility, SF		No. of Subproblems	
		Algorithm 2	Sequential	Algorithm 2	Sequential
(10,2)	32	0.6010	0.6089	1 mp-NLP	33 NLPs
	64	0.6010	0.6089	+ 2 mp-LPs	65 NLPs
(12,2)	32	0.8486	0.8534	No	33 NLPs
	64	0.8487	0.8535	Extra	65 NLPs
(14,2)	32	0.9999	0.9999	No	33 NLPs
	64	0.9999	0.9999	Extra	65 NLPs
(10,3)	32	0.5687	0.5762	No	33 NLPs
	64	0.5687	0.5762	Extra	65 NLPs
(10,4)	32	0.5363	0.5426	No	33 NLPs
	64	0.5363	0.5426	Extra	65 NLPs
			Total:	1 mp-NLP + 2 mp-LPs	490 NLPs

lems with a large number of uncertain parameters, since even for an intermediate number, the sequential approach explodes (for an example of this, see Table 7 in Bansal et al., 2000).

Note that the use of the feasibility function expressions in Step 2a of Algorithm 2 can lead to the individual optimization subproblems having a higher number of constraints compared to existing approaches where the process inequalities are used. This is seen for the illustrative example where there are three process inequalities (Eq. 16) but nine approximating linear feasibility function expressions (Eqs. 17–25). However, this effect is insignificant compared to the reduction in the number of subproblems, as described earlier. The use of the feasibility function expressions in Algorithm 2 also has the desirable consequence that the subproblems in Step 2a become linear.

(3) For the evaluation of the $ESF(\boldsymbol{d})$, defined in Eq. 11 as

$$ESF(\boldsymbol{d}) = \sum_{s=S_1}^{2^{eq}} SF(\boldsymbol{d}, \boldsymbol{y}^s) \cdot P(\boldsymbol{y}^s)$$

all the advantages of Algorithm 2 just described will be carried over, since it relies on a stochastic flexibility evaluation for each system state.

New Framework for Flexibility Analysis and Design

Based on the theoretical development presented in Bansal et al. (2000) and in this article, we are now able to propose a unified, conceptual framework for the flexibility analysis and design optimization of linear or nonlinear systems with deterministic or stochastic parameters. The new framework is illustrated in Figure 7. Note that the framework incorporates both convex and nonconvex models; in principle, the flexibility analysis and design of nonconvex systems can be achieved using similar ideas to those presented for convex systems (see Bansal (2000) for detailed algorithms).

For both linear and nonlinear systems, the common starting point in the framework is to solve the feasibility function problem (Eq. 5) as a multiparametric program using specialized algorithms. This gives a set of linear expressions for the feasibility function in terms of $\boldsymbol{\theta}$, $\boldsymbol{d}$, and $\boldsymbol{y}$, which are exact for linear systems and globally accurate within a user-specified tolerance for nonlinear systems, and an associated set of regions in which these solutions are optimal. For systems with deterministic parameters, the critical values of the uncertain parameters can be identified through vertex properties for linear and convex models and through the solution of further multiparametric linear programs for nonconvex models. It is then possible to express the feasibility test measure, χ, and the flexibility index, F, as explicit linear functions of the design variables. This reduces their evaluation to simple function evaluations for a given design and enables a designer to know *a priori* the regions in the design space for which feasible operation can be guaranteed.

The critical parameter information and the expressions for χ and F can be used to formulate design optimization problems that, unlike existing approaches, do not require iteration between a design step and a flexibility analysis step. Instead, the optimal design for a fixed degree of flexibility is determined through the solution of a single (mixed-integer) nonlinear program, while the algebraic form of the trade-off curve of cost against flexibility index can be generated explicitly by solving a single-parameter (mixed-integer), nonlinear program.

For systems with stochastic parameters described by any probability distribution, the procedures for evaluating the stochastic flexibility and the expected stochastic flexibility metrics are identical for both linear and nonlinear models once the parametric feasibility function expressions have been generated. The use of these expressions is especially significant for nonlinear systems because they remove all nonlinearity from the intermediate optimization subproblems, something that would not be possible using nonparametric approaches. Furthermore, by considering the subproblems as multiparametric linear programs, the number of problems that needs to solved compared to existing approaches is drastically reduced and parametric information is obtained that allows the metrics to be evaluated for any design through a series of function evaluations.

Concluding Remarks

This article has described a new framework for conducting flexibility analysis and design optimization under uncertainty. The framework provides a unified-solution approach, based on parametric programming, for different types of process

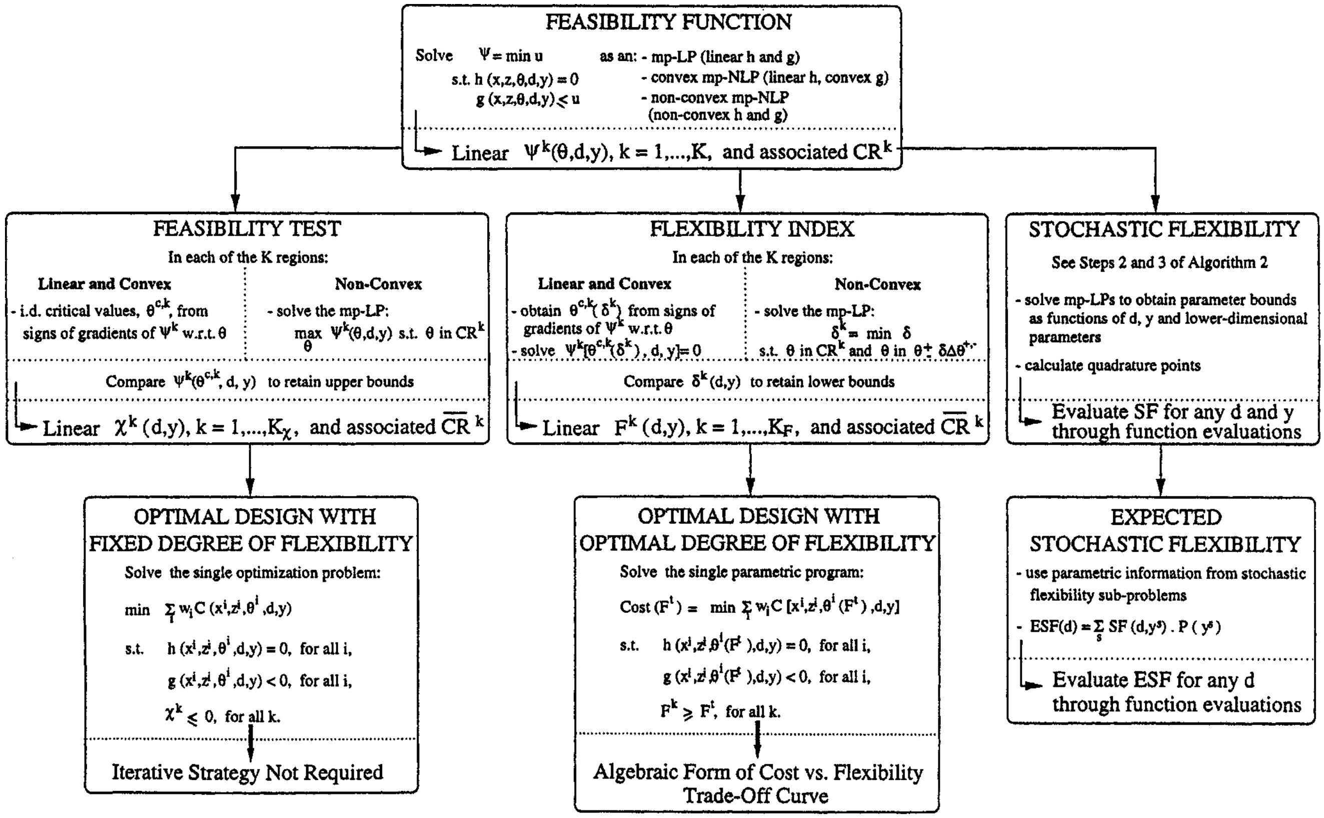

Figure 7. Unified parametric programming framework for flexibility analysis and design.

model (linear, convex, and nonconvex) and different types of uncertainty (deterministic and stochastic). For steady-state systems discribed by general classes of models, the framework:

- Allows the critical values of the uncertain parameters that limit flexibility to be identified *a priori*.
- Gives the feasibility test measure and flexibility index as explicit functions of the design variables.
- Reduces the feasibility test and index problems to simple function evaluations for a given design.
- Allows a designer to know in advance for which designs feasible operation will be possible in the face of the specified uncertainties.
- Enables design optimization problems to be solved without having to iterate between a design step and a flexibility analysis step.
- Gives the algebraic form of the trade-off curve of cost against flexibility index.
- Involves linear optimization subproblems during stochastic flexibility evaluation, even for nonlinear process models.
- Has a linear rather than exponential increase in the number of optimization subproblems that need to be solved as the number of uncertain parameters increases in stochastic flexibility problems.
- Allows the stochastic and expected stochastic flexibility to be evaluated for a given design and number of quadrature points through a simple series of function evaluations.

The framework can also accommodate the analysis and design of other systems. For example, as described in Bansal et al. (2001), for an in-line blending system where some of the control variables are binary variables corresponding to discrete modes of operation, the starting feasibility function problem in the framework of Figure 7 corresponds to a multiparametric, mixed-integer linear program (mp-MILP). An algorithm such as that of Acevedo and Pistikopoulos (1999) or Dua and Pistikopoulos (2000) can be used to obtain linear parametric expressions for the feasibility functions, and then the various flexibility analysis and design problems can be tackled using the framework in a similar manner to that already described. This will be the subject of a future article. Bansal (2000) also discusses the potential for using an analogous framework for the analysis, design, and control optimization of dynamic systems under uncertainty if methods could be developed for solving multiparametric (mixed-integer), dynamic optimization, or mp-(MI)DO problems.

Finally, as referred to earlier in the article, ongoing research is aimed at improving the efficiency of the underlying parametric programming algorithms, particularly those for nonconvex mp-NLPs, in order to enable larger, more realistic problems to be solved.

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Appendix: An Algorithm for Convex mp-NLPs

Description

An algorithm for the solution of convex mp-MINLPs was proposed by Dua and Pistikopoulos (1999). Here, the primal part of this algorithm, for the solution of convex mp-NLPs, is outlined, with some slight modifications to make it more amenable for flexibility analysis problems.

Consider a problem of the general form

$$\begin{aligned} \text{Obj}\ (\boldsymbol{\Theta}) = \min_{\boldsymbol{w}}\ & c^{\text{convex}}(\boldsymbol{w}) \\ \text{s.t.}\quad & \mathbf{0} = \boldsymbol{h}^{\text{linear}}(\boldsymbol{w},\boldsymbol{\Theta}) \\ & \mathbf{0} \geq \boldsymbol{g}^{\text{convex}}(\boldsymbol{w},\boldsymbol{\Theta}) \\ & \boldsymbol{\Theta}^{L} \leq \boldsymbol{\Theta} \leq \boldsymbol{\Theta}^{U} \end{aligned} \tag{A1}$$

where $\boldsymbol{w}$ is a vector of search variables and $\boldsymbol{\Theta}$ is a vector of parameters.

(1) Find an initial feasible point. This can be accomplished, for example, by solving Eq. A1, with $\boldsymbol{\Theta}$ treated as search variables along with $\boldsymbol{w}$. If there is no solution, the problem is infeasible; otherwise, a feasible solution $(\boldsymbol{w}^*,\boldsymbol{\Theta}^*)$ is found.

(2) (a) Create an outer approximation of Eq. A1 by linearizing the nonlinear functions c^{convex} and $\boldsymbol{g}^{\text{convex}}$ at $(\boldsymbol{w}^*,\boldsymbol{\Theta}^*)$. This gives

$$\begin{aligned} \check{Obj}\ (\boldsymbol{\Theta}) = \min_{\boldsymbol{w}} & \left[c^{\text{convex}}(\boldsymbol{w}^*) + \nabla_{w}\cdot c^{\text{convex}}(\boldsymbol{w}^*)\cdot(\boldsymbol{w}-\boldsymbol{w}^*)\right] \\ \text{s.t.}\quad & \mathbf{0} = \boldsymbol{h}^{\text{linear}}(\boldsymbol{w},\boldsymbol{\Theta}) \\ & \mathbf{0} \geq \boldsymbol{g}^{\text{convex}}(\boldsymbol{w}^*,\boldsymbol{\Theta}^*) + \nabla_{w}\cdot \boldsymbol{g}^{\text{convex}}(\boldsymbol{w}^*,\boldsymbol{\Theta}^*)\cdot(\boldsymbol{w}-\boldsymbol{w}^*) \\ & \quad + \nabla_{\Theta}\cdot \boldsymbol{g}^{\text{convex}}(\boldsymbol{w}^*,\boldsymbol{\Theta}^*)\cdot(\boldsymbol{\Theta}-\boldsymbol{\Theta}^*) \\ & \boldsymbol{\Theta}^{L} \leq \boldsymbol{\Theta} \leq \boldsymbol{\Theta}^{U} \end{aligned} \tag{A2}$$

(b) Solve Eq. A2 as an mp-LP using the algorithm of Gal and Nedoma (1972) described in Appendix A of Bansal et al. (2000). This will give a set of linear expressions, $\check{Obj}$ $(\boldsymbol{\Theta})$, and a corresponding set of regions, defined by linear inequalities in $\boldsymbol{\Theta}$, in which these solutions are optimal.

(3) Since *Obj* $(\boldsymbol{\Theta})$ is a convex function of $\boldsymbol{\Theta}$, the point of maximum discrepancy between the linear solution $\check{Obj}$ $(\boldsymbol{\Theta})$ and *Obj* $(\boldsymbol{\Theta})$ in each region of optimality will lie at one of the vertices of the region. Therefore:

(a) Identify all the feasible vertices of the regions of optimality found in Step 2b. In order to achieve this, Dua and Pistikopoulos (1999) used an iterative procedure based on fixing some of the inequalities that describe each region; solving the resulting square system of linear equations; testing whether the solution satisfies the "unfixed" inequalities and storing that vertex if they do; and repeating this for all square combinations of active inequalities. Here, we propose an alternative strategy. In each region of optimality, first a mixed-integer linear program (MILP) is solved with a dummy objective function, corresponding to:

$$\begin{aligned} & \min_{\boldsymbol{\Theta}}\ \mathbf{0}^{T}\cdot\boldsymbol{\Theta} \\ \text{s.t.}\quad & CR_i^k(\boldsymbol{\Theta}) + s_i^k = 0, \quad \forall i \\ & s_i^k - U(1-p_i^k) \leq 0, \quad \forall i \\ & \sum_i p_i^k = n_{\Theta} \\ & p_l = 0,1;\ s_l \geq 0, \quad \forall_i \end{aligned} \tag{A3}$$

In Eq. A3 CR_i^k $(\boldsymbol{\Theta}) \leq 0$ is the ith inequality defining the kth region CR^k; s_i^k are positive slack variables with an upper bound of U; p_i^k is a binary variable that takes a value of 1 if inequality i is active ($CR_i^k = 0$), and is zero otherwise; and n_{Θ} is the number of elements in the vector of parameters $\boldsymbol{\Theta}$.

Once Eq. A3 has been solved to give a vertex, two sets are formed. The first, I^a, consists of the integers associated with the active inequalities, while the second, I^{na}, corresponds to the set of inactive inequalities, that is, $I^a = \{i|y_i^k = 1\}$ and $I^{na} = \{i|y_i^k = 0\}$. Equation A3 is then re-solved with the addition of the integer cut

$$\sum_{i\in I^a} y_i^k - \sum_{i \in I^{na}} y_i^k \leq n_{\Theta} - 1 \tag{A4}$$

to exclude the previous vertex solution. This procedure is repeated until Eq. A3 becomes infeasible, at which point all the feasible vertices have been identified.

It should be noted that any other vertex enumeration algorithm can be used in the preceding step if it is found to be more efficient. Other vertex enumeration algorithms have been proposed by, for example, Bremner et al. (1998).

(b) At each of the V^k vertices, $\boldsymbol{\Theta}^{v,k}$, in the kth region of optimality, evaluate the difference, $Obj_{\text{diff}}^{v,k}$ between the actual objective function *Obj* $(\boldsymbol{\Theta}^{v,k})$ and the linear underestimator $\check{Obj}$ $(\boldsymbol{\Theta}^{v,k})$. If, for any of the vertices in any of the regions, $Obj_{\text{diff}}^{v,k} > \epsilon$, where ϵ is a user-specified tolerance, Step 2a is returned to the vertex that gives the worst discrepancy as the point for linearization. The parametric expressions resulting from the solution of the new np-LP in Step 2b are compared with the previous linear solutions using the procedure of Acevedo and Pistikopoulos (1997b), as described in Appendix B of Bansal et al. (2000), so as to retain the tighter underestimators, and a new set of regions of optimality is defined. The vertices are identified, and so on, until $Obj_{\text{diff}}^{v,k} \leq \epsilon$, $\forall v$, $\forall k$.

(4) The final underestimators resulting from Step 3b are converted to overestimators. Dua and Pistikopoulos (1999) proposed the addition of ϵ to each expression. Alternatively, slightly tighter overestimators can potentially be obtained by adding

$$\bar{\epsilon} = \max_{v,k}\ \left(Obj_{\text{diff}}^{v,k}\right) \tag{A5}$$

The regions of optimality remain unchanged.

Illustrative example

Consider the feasibility function problem for the system, Eq. 16, where $\boldsymbol{w} = [z,u]^T$, $\boldsymbol{\Theta} = [\theta_1,\theta_2,d_1,d_2]^T$, $\boldsymbol{\Theta}^L = [1.5,1.5,10,2]^T$ and $\boldsymbol{\Theta}^U = [4.5,4.5,15,4]^T$. Set $\epsilon = 0.005$.

(1) A feasible point, $\boldsymbol{\Theta}^{*,1} = [1.5,1.5,10,2]^T$, is obtained, with corresponding $\boldsymbol{w}^{*,1} = [11.4582, -0.4331]^T$.

(2) The outer approximation problem for this example is

$$\check{\psi}(\boldsymbol{\theta},\boldsymbol{d}) = \min_{z,u} u$$

$$\text{s.t.} \quad u \geq -0.08(z^*)^2 + 0.16z^*z - \theta_1 - \frac{1}{20}\theta_2 + \frac{1}{5}d_1 - 13$$

$$u \geq -z - \frac{1}{6}(\theta_1^*)^{1/2} - \frac{1}{6}(\theta_1^*)^{-1/2}\theta_1 + \frac{1}{20}d_2 + 11\frac{1}{3} \quad \text{(A6)}$$

$$u \geq e^{0.21z^*}\cdot[1 + 0.21(z - z^*)] + \theta_1 - \frac{1}{20}\theta_2 - \frac{1}{5}d_1 - \frac{1}{20}d_2 - 11$$

$$1.5 \leq \theta_1, \quad \theta_2 \leq 4.5$$

$$10 \leq d_1 \leq 15$$

$$2 \leq d_2 \leq 4$$

Solving Eq. A6 as an mp-LP at $\boldsymbol{\Theta}^{*,1}$ and $\boldsymbol{w}^{*,1}$ gives

$$\check{\psi}^1(\boldsymbol{\theta},\boldsymbol{d}) = 0.2052\theta_1 + 0.0150\theta_2 - 0.0601d_1 + 0.0200d_2 - 0.2025, \quad \text{(A7)}$$

$$CR^1 = \begin{cases} 1.5 \leq \theta_1, \quad \theta_2 \leq 4.5 \\ 10 \leq d_1 \leq 15 \\ 2 \leq d_2 \leq 4 \end{cases}$$

(3) The vertices in CR^1 simply correspond to the 16 vertices in $\theta_1 - \theta_2 - d_1 - d_2$ space. The worst one is $\boldsymbol{\Theta} = [4.5,4.5,10,2]^T$, where $\psi = 0.3895$, $\check{\psi}^1 = 0.2274$, and, thus, $\psi_{\text{diff}}^1 = 0.1621$.

(4) Solving Eq. A6 at $\boldsymbol{\Theta}^{*,2} = [4.5,4.5,10,2]^T$ and $\boldsymbol{w}^{*,2} = [10.3367,0.3895]^T$ gives

$$\check{\psi}^2(\boldsymbol{\theta},\boldsymbol{d}) = 0.3011\theta_1 + 0.0176\theta_2 - 0.0704d_1 + 0.0148d_2 - 0.3703 \quad \text{(A8)}$$

(5) Comparing $\check{\psi}^1$ and $\check{\psi}^2$ in order to retain the tighter underestimators leads to two new regions of optimality

$$\check{\psi}^1(\boldsymbol{\theta},\boldsymbol{d}) = 0.2052\theta_1 + 0.0150\theta_2 - 0.0601d_1 + 0.0200d_2 - 0.2025$$

$$CR^1 = \begin{cases} 37.1436\theta_1 + \theta_2 - 4d_1 - 2d_2 \leq 64.9242 \\ 1.5 \leq \theta_1 \\ 1.5 \leq \theta_2 \leq 4.5 \\ 10 \leq d_1 \leq 15 \\ 2 \leq d_2 \leq 4 \end{cases}$$

$$\check{\psi}^2(\boldsymbol{\theta},\boldsymbol{d}) = 0.3011\theta_1 + 0.0176\theta_2 - 0.0704d_1 + 0.0148d_2 - 0.3703$$

$$CR^2 = \begin{cases} 37.1436\theta_1 + \theta_2 - 4d_1 - 2d_2 \geq 64.9242 \\ \theta_1 \leq 4.5 \\ 1.5 \leq \theta_2 \leq 4.5 \\ 10 \leq d_1 \leq 15 \\ 2 \leq d_2 \leq 4 \end{cases}$$

(6) Solving the MLP (43) with integer cuts gives Table A1. $\boldsymbol{\Theta} = [1.5,1.5,15,4]^T$ in CR^1 is, thus, chosen as the next point for linearization.

(7) Solving Eq. A6 at $\boldsymbol{\Theta}^{*,3} = [1.5,1.5,15,4]^T$ and $\boldsymbol{w}^{*,3} = [11.7170, -0.5919]^T$ gives

$$\check{\psi}^3(\boldsymbol{\theta},\boldsymbol{d}) = -0.4366\theta_1 - 0.0174\theta_2 + 0.0696d_1 + 0.0326d_2 - 1.0849 \quad \text{(A9)}$$

(8) Comparing $\check{\psi}^1$, $\check{\psi}^2$, and $\check{\psi}^3$ leads to the new regions of optimality

$$\check{\psi}^1(\boldsymbol{\theta},\boldsymbol{d}) = 0.2052\theta_1 + 0.0150\theta_2 - 0.0601d_1 + 0.0200d_2 - 0.2025$$

$$CR^1 = \begin{cases} 37.1436\theta_1 + \theta_2 - 4d_1 - 2d_2 \leq 64.9242 \\ -19.8006\theta_1 - \theta_2 + 4d_1 + 0.3901d_2 \leq 27.2249 \end{cases}$$

$$\check{\psi}^2(\boldsymbol{\theta},\boldsymbol{d}) = 0.3011\theta_1 + 0.0176\theta_2 - 0.0704d_1 + 0.0148d_2 - 0.3703$$

$$CR^2 = \{37.1436\theta_1 + \theta_2 - 4d_1 - 2d_2 \geq 64.9242$$

$$\check{\psi}^3(\boldsymbol{\theta},\boldsymbol{d}) = -0.4366\theta_1 - 0.0174\theta_2 + 0.0696d_1 + 0.0326d_2 - 1.0849$$

$$CR^3 = \{-19.8006\theta_1 - \theta_2 + 4d_1 + 0.3901d_2 \geq 27.2249$$

where simple bounds have been omitted for clarity.

Table A1. Solving MILP with Integar Cuts

k	No. Vertices in CR^k	Worst Vertex	ψ	$\check{\psi}^k$	ψ_{diff}^k
1	16	$[1.5,1.5,15,4]^T$	−0.5919	−0.6935	0.1016
2	16	$[3.5383,1.5,15,4]^T$	−0.2268	−0.2754	0.0486

Table A2. Vertex Identification

k	No. Vertices in CR^k	Worst Vertex	ψ	$\check{\psi}^k$	ψ_{diff}^k
1	21	$[3.5383,1.5,15,4]^T$	−0.2268	−0.2754	0.0486
2	16	$[3.5383,1.5,15,4]^T$	−0.2268	−0.2754	0.0486
3	11	$[1.6583,1.5,15,4]^T$	−0.6539	−0.6610	0.0071

(9) The results of the vertex identification and comparison in the three regions are given in Table A2. $\boldsymbol{\Theta}^{*,4} = [3.5383,1.5,15,4]^T$, on the boundary of CR^1 and CR^2, is chosen as the next point at which to solve the outer approximation problem. The procedure illustrated is repeated until eventually nine linear underestimators for ψ are found where all vertices of their associated regions of optimality give discrepancies of less than $\epsilon = 0.005$. The maximum discrepancy, $\bar{\epsilon}$, is actually 0.0042 and occurs at the vertex $[3.9258,4.5,10,2]^T$ where $\check{\psi}^2 = \check{\psi}^6$. After the addition of $\bar{\epsilon} = 0.0042$, the overestimating solutions, Eqs. 17–25, result.

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