New Approach for Quantifying Process Feasibility: Convex and 1-D Quasi-Convex Regions

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Uncertainities in chemical plants come from numerous sources: internal like fluctuated values of reaction constants and physical properties or external such as quality and flow rates of feedstreams. Accounting for uncertainty in various stages of plant operations was identified as one of the most important problems in chemical plant design and operations. A new approach proposed describes process's feasible region and a new metric for evaluating process flexibility based on the convex hull that is inscribed within the feasible region and determines its volume based on Delaunay Triangulation. The two steps involved are: 1. a series of simple optimization problems are solved to determine points at the boundary of the feasible region; 2. given the set of points at the boundary of the feasible region, the convex hull inscribed within the feasible region is determined. This is achieved by implementing the Quickhull algorithm, an incremental procedure for evaluating the convex hull, and then by computing a Delaunay Triangulation to determine the volume of the convex hull providing a new metric for process flexibility. This approach not only provides another feasibility measure, but an accurate description of the feasible space of the process. It was applied to 1-D convex problems, and work is in progress to extend it to nonconvex systems.

Introduction

Production systems typically involve significant *uncertainty* in their operation. Variability of process parameters during operation and plant model mismatch (both parametric and structural) could give rise to suboptimality and even infeasibility of the deterministic solutions. Consequently, plant flexibility has been recognized to represent one of the important components in the operability of the production processes.

A brief overview of the approaches that exist in the literature to deal with the problem of feasibility and flexibility quantification follows in this section.

In a broad sense the area covers (i) *a feasibility test* that requires constraint satisfaction over a specified space of uncertain parameters, (ii) a *flexibility index* associated with a given design that represents a quantitative measure of the range of uncertainty space that satisfies the feasibility temperature, and (iii) the integration of design and operations where trade-offs between design cost and plant flexibility are considered.

Halemane and Grossmann (1983) proposed a feasibility measure for a given design based on the worst points for feasible operation, which can be mathematically formulated as a *max-min-max optimization problem* as follows

$$\chi(d) = \max_{\theta \in T} \min_{z} \max_{j \in],\, i \in I} \left\{ h_i(d, z, x, \theta) = 0;\ g_j(d, z, x, \theta) \le 0 \right\}, \qquad (1)$$

where the function $\chi(d)$ represents a feasibility measure, d corresponds to the vector of design variables, z the vector of control variables, x the vector of state variables, and θ the vector of uncertain parameters. If $\chi(d) \le 0$, design d is feasible for all $\theta \in T$, whereas if $\chi(d) > 0$, the design cannot operate for at least some values of $\theta \in T$.

The above mass-min-max problem defines a nondifferentiable global optimization problem, which, however, can be reformulated as the following two-level optimization problem

$$\chi(d) = \max_{\theta \in T} \psi(d, \theta)$$

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

$$\text{s.t. } h_i(d, z, x, \theta) = 0; \; i \in I$$

$$g_j(d, z, x, \theta) \le u \quad j \in J, \tag{2}$$

where the function $\psi(d, \theta) = 0$ defines the boundary of the feasible region in the space of the uncertain parameters θ.

The design flexibility index problem as introduced by Swaney and Grossmann (1985a) can be reformulated to represent the determination of the largest hyperrectangle that can be inscribed within the feasible region of the design. Following this idea, the mathematical formulation of the flexibility problem has the following form

$$F = \min \delta$$

$$\text{s.t. } \psi(d, \theta) = 0$$

$$\psi(d, \theta) = \min_z u$$

$$h_i(d, z, x, \theta) = 0, \quad i \in I$$

$$g_j(d, z, x, \theta) \le u, \quad j \in J$$

$$T(\delta) = \{\theta \mid \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N - \delta\Delta\theta^+\}$$

$$\delta \ge 0. \tag{3}$$

Other approaches that exist in the literature to quantify the flexibility for a given design involve the deterministic measures such as the Resilience Index (RI), proposed by Saboo et al. (1983), the flexibility index proposed by Swaney and Grossmann (1985a,b) and the stochastic measures such as the design reliability proposed by Kubic and Stein (1988), the stochastic flexibility index proposed by Pistikopoulos and Mazzuchi (1990) and Straub and Grossmann (1983).

For the case where the constraints are one-dimensional (1-D) jointly quasi-convex in θ and quasi-convex in z, it was proven by Swaney and Grossmann (1985a) that the point θ_c that defines the solution to Eq. 2 lies at one of the vertices of the parameter set T. Based on this assumption, the critical uncertain parameter points correspond to the vertices and the feasibility test problem is reformulated in the following manner

$$\chi(d) = \max_{k \in V} \psi(d, \theta^k), \tag{4}$$

where $\psi(d, \theta^k)$ is the evaluation of the function $\psi(d, \theta)$ at the parameter vertex θ^k and V is the index set for the 2^{n_p} vertices for the n_p uncertain parameters θ. In a similar fashion for the flexibility index, problem 3 is reformulated in the following way

$$F = \min_{k \in V} \delta^k, \tag{5}$$

where δ^k is the maximum deviation along each vertex direction $\Delta\theta^k$, $k \in V$ and is determined by the following problem

$$\delta^k = \max_{\delta, z} \delta$$

$$\text{s.t. } g_j(d, z, x, \theta) \le 0, \; j \in J$$

$$h_i(d, z, x, \theta) = 0, \; i \in I$$

$$\theta = \theta^N + \Delta\theta^k, \; \delta \ge 0. \tag{6}$$

Based on the above problem reformulations, Halemane and Grossmann (1983) proposed the direct search method that explicitly enumerates all the parameter set vertices. To avoid the explicit vertex enumeration, Swaney and Grossmann (1985a,b) proposed two algorithms, a heuristic vertex search, and an implicit enumeration scheme. These algorithms rely on the assumption that the critical points correspond to the vertices of the parameter set T which is valid if the constraints are jointly 1-D quasi-convex in θ and quasi-convex in z. To circumvent this limitation, Grossmann and Floudas (1987) proposed a solution approach based on the following ideas:

(a) They replace the inner optimization problem by the *Karush Kuhn, Tucker optimality conditions* (KKT);

(b) They utilize the discrete nature of the selection of the active constraints by introducing a set of binary variables to express if a specific constraint is active.

Based on these ideas, the feasibility test and flexibility index problems can be reformulated as *mixed-integer optimization problems* either linear or nonlinear depending on the nature of the constraints. Grossmann and Floudas (1987) proposed the active set strategy for the solution of the above reformulated problems based on the property that for any combination of $n_z + 1$ binary variables that is selected (that is, for a given set of active constraints), all the other variables can be determined as a function of θ. They proposed a procedure of systematically identifying the potential candidates for the active sets based on the signs of the gradients $\nabla_z g_j(d, z, x, \theta)$. Ostrovky et al. (1994) proposed a branch and bound approach based on the evaluation of the upper and lower bound of function $\chi(d)$. Although the suggested bounding problems are simpler than the original feasibility test problem, they correspond to bilevel optimization problems where global optimality cannot be guaranteed using local optimization methods (Migdalas et al., 1998). Finally, a global optimization approach is proposed recently by Floudas et al. (2000) to guarantee the determination of the global optimal solution for both the feasibility and the feasibility index problem by generating a relaxation/enlargement of the feasible region based on the convexification of the original problem constraints.

Following this introduction, a small example is studied in the next section to motivate the need of developing a new approach for quantifying the range of feasibility for a given process. The new approach and the detailed procedure that we propose is introduced to determine the new metric that describes the feasible region. The motivating example is used to illustrate the basic steps of the proposed approach and the results obtained. Several examples from the literature are covered and compared with the results of the previously used approaches. The extension of the basic framework to cover 1-D convex regions is discussed and the basic advantages of the proposed approach are summarized.

Motivating Example

The example presented here is a modification of example 2 used by Pistikopoulos and Ierapetritou (1995). The design is described by two parameters (d_1, d_2) whereas z_1, z_2 are the control variables and θ_1, θ_2 are the uncertain parameters. The constraints of the problem are the following

$$f_1 = -1.3 + 1.6 \times \theta_1 - 1.6 \times z_1 + 2.14 z_2 \leq 0$$
$$f_2 = \theta_1^2 - 2.5\theta_2 + 12 \times z_1 - 2 z_2 \leq 0$$
$$f_3 = 2.61 \times z_1 - d_1 \leq 0$$
$$f_4 = 3.14 \times z_2 - d_2 \leq 0$$
$$f_5 = -z_1 \leq 0$$
$$f_6 = -z_2 \leq 0$$
$$0 \leq \theta_1 \leq 2$$
$$0 \leq \theta_2 \leq 8.$$

The design examined first corresponds to $d_1 = 3.5$, $d_2 = 0.0$. For this problem, first the active sets are identified based on the fact that three constraints should be active at a time since there are two control variables (Grossmann and Floudas, 1987)

$$\text{Active Set } 1 = \{f_1, f_2, f_3\}$$
$$\text{Active Set } 2 = \{f_1, f_2, f_5\}$$
$$\text{Active Set } 3 = \{f_1, f_2, f_6\}$$
$$\text{Active Set } 4 = \{f_1, f_2, f_4\}$$
$$\text{Active Set } 5 = \{f_1, f_3, f_6\}$$
$$\text{Active Set } 6 = \{f_2, f_4, f_5\}$$

For each one of these active sets, the feasibility function is determined and plotted in Figure 1. The flexibility index problem is then solved using the active set strategy approach proposed by Grossmann and Floudas (1987) that results in a value of F = 0.278. This value describes the rectangular which is shown dark shaded in Figure 1.

Note that, although the actual feasible region of the design is the light shaded region, the flexibility index identifies only a small percentage of it and thus it largely underestimates design's feasibility. Moreover, the flexibility index does not provide always accurate results for comparing different designs. For example, we are considering next the design that corresponds to $d_1 = 2.5$, $d_2 = 3.5$. For this design, the feasible region is evaluated based on the determination of the different active sets. The results are illustrated in Figure 2. Note that this design has a smaller feasible region since active set 5 constraint moved to the left and thus the design's feasible region is more restricted. However, the flexibility of this design is F = 0.278, the same as for the design 1.

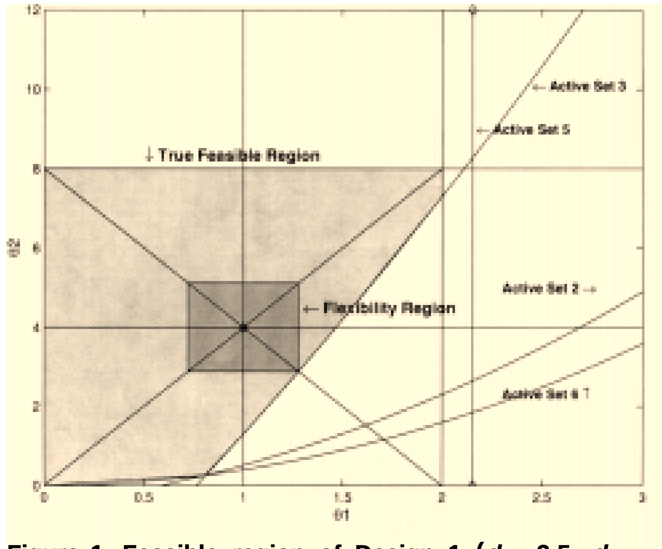

Figure 1. Feasible region of Design 1 ($d_1 = 3.5$, $d_2 = 0.0$).

The results presented for the specific example clearly motivate the need of developing a new approach for determining the feasibility range for a given process and a new metric for evaluating its flexibility that can be used for comparison between designs.

Proposed Approach

To illustrate the basic concept of the proposed approach, let's assume that the specific design is described by a set of inequality constraints $f_j(d, z, \theta) \leq 0$ assuming that the equality constraints have been eliminated for ease in the presentation. In these constraints d represents the set of design variables, and z the set of control variables that can be adjusted to accommodate variations on the uncertain parameter vector θ. Following the ideas of Grossmann and Halemane (1982), one can map the feasible region into the uncertainty

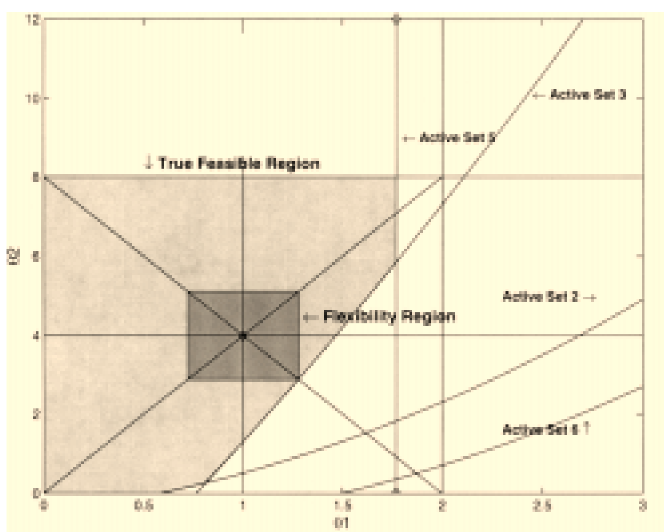

Figure 2. Feasible region of Design 2 ($d_1 = 2.5$, $d_2 = 3.5$).

space by evaluating the feasibility function

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

$$f_j(d,z,\theta) \le u, \forall j \in J.$$

Alternatively, the same result can be obtained by identifying all the active constraint sets. The question that arises at this stage in many different engineering problems is how to describe and then quantify the feasible range.

The first case that we are going to address is the convex case, the extension to the 1-D convex case will be discussed later. The main idea in the proposed approach is first to determine points at the boundary of the feasible region and then to evaluate the convex hull defined by those points. For the case of the convex feasible region, the convex hull determined in this way is guaranteed to be inscribed within the feasible region. However, for the nonconvex case, there is no guarantee that this would be always the case. To overcome this difficulty, an extension of the basic proposed approach is presented later whereas the general nonconvex case would be the subject of future publication. For the convex case, the following steps are considered:

(1) Solve the problems of determining the maximum deviation from the nominal point towards the vertices $(k \epsilon K)$ of the expected range of uncertain parameter (θ_i) variability

$$\max \delta^k$$
$$\text{s.t. } f_j(d,z,\theta_i) \le 0,\ j \in J$$
$$\theta_i = \theta_i^N \pm \delta^k \Delta \theta_i^{\pm}$$

(2) Solve the problems of determining the maximum deviation from the nominal point by varying one uncertain parameter (θ_i) at a time

$$\max \delta_i$$
$$\text{s.t. } f_j(d,z,\theta_1,\theta_2) \le 0,\ j \in J$$
$$\theta_i = \theta_i^N \pm \delta \Delta \theta_i^{\pm}$$
$$\theta_j = \theta_j^N \forall j \ne i$$

(3) Determine the convex hull based in the points obtained from steps (1) and (2) applying the *Quickhull algorithm* which is described below.

(4) Determine the volume of the convex hull obtained from step (3) using *Delaunay Triangulation* (the basics of the *Delanay Triangulation* are explained in the sequel). At the same step and using the vertices of the expected range of uncertain parameter variability, the volume of the overall expected region is determined. The ratio between the feasible convex hull and the expected region ''volumes'' is then evaluated to represent the new metric for comparing design's feasibility

$$\text{Feasible Convex Hull Ratio (FCHR)} = \frac{\text{Volume of the feasible convex hull}}{\text{Volume of the overall expected range}} \quad (7)$$

Note that, at step 3, the linear functions describing the faces of the convex hull are also determined. As will be illustrated by different examples, this provides a very accurate description of the feasible space for a specific design or process which is of great importance in many different engineering problems. An example is the determination of the range of validity of a reduced kinetic model as described by Androulakis et al. (2000).

Quickhull algorithm

The convex hull of a set of points is the smallest convex set that contains the points. There exist a number of different algorithms in the computational geometry literature that are designed to compute the convex hull for a given set of points. A review can be found in de Berg et al. (1997). Recent work on convex hull has been focused on variations of a randomized, incremental algorithm where points are considered one at a time. *Quickhull algorithm* (Barber et al., 1996) proceeds using two geometric operations: oriented hyperplane through (n_d) points and signed distance to hyperplane. In particular the following steps are followed for each processed point:

(a) Locate the visible facets for the point. A facet is visible if the point is above the facet. The selection is made by evaluating the signed distance from the facet;

(b) Construct a cone of new facets from the point to the visible facets;

(c) Delete the visible facets thus forming the convex hull of the new point and the previous processed points.

The correctness of the algorithm has been proved by Barber et al. (1996). They also provide empirical evidence that the algorithm runs faster when the input set of points contains no extreme points. The detailed description of the algorithm, as well as the programming implementation, can be found and downloaded from the Web site of the geometry center in Minneapolis: http://www.geom.umn.edu/software/download.

Delaunay triangulation

The basic definition of the *Delauany Triangulation* is the graph that has a node for every *Voronoi cell* and a straight line connecting two nodes if the corresponding cells share an edge. The *Voronoi diagram* of a set of points (n) is the subdivision of the plate into (n) regions one for each site such that the region of a specific site contains all the points in the plane for which this site is the closest. The region of this site is called the *Voronoi cell*. The computation of the *Delaunay Triangulation* is based on the same iterative procedure as the convex hull estimation. In particular, a *Delaunay Triangulation* in R^d can be computed from a convex hull in R^{d+1}, as described by Barber et al. (1996). The same software described above has the capability of evaluating Delaunay Triangulation.

Example revisited

The example presented in the previous section is used here again to illustrate the basic steps of the proposed approach and the results obtained. The problem involves convex constraints so there is no need for function convexification. The

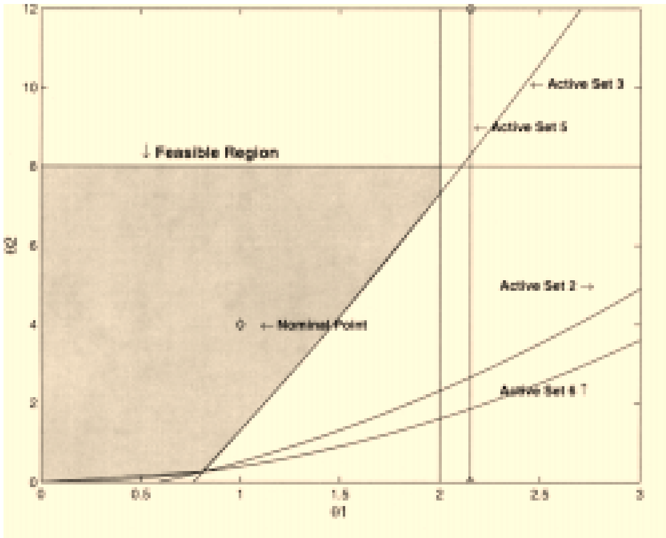

Figure 3. Feasible region of Design 1 ($d_1 = 3.5$, $d_2 = 0.0$).

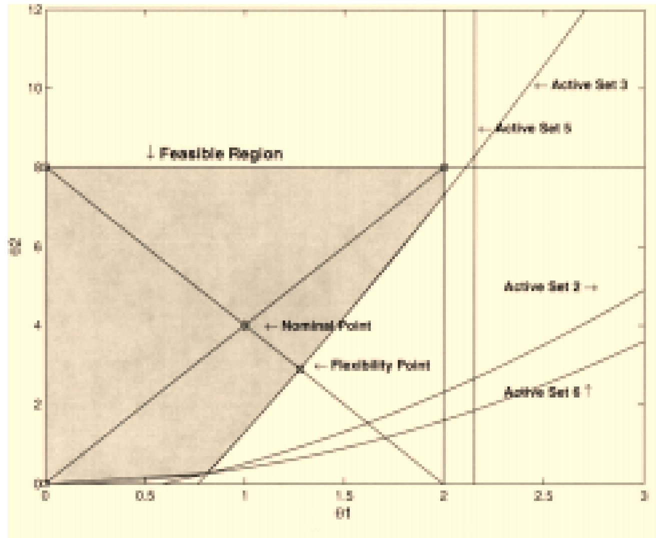

Figure 4. Step 1: finding points at the boundary (vertices).

active sets of the problem have been identified and the feasible region is described by the shaded region shown in Figure 3.

The steps of the proposed analysis are then followed.

Step 1. Solve the optimization problems of maximizing the deviations from the nominal point towards the edges. The problems solved have the following form

$$\max \delta^i$$
$$\text{s.t. } f_j(d, z, \theta_1, \theta_2) \le 0, \; j = 1, \ldots, 6$$
$$\theta_1 = \theta_1^N \pm \delta^i \Delta\theta_1^{\pm}$$
$$\theta_2 = \theta_2^N \pm \delta^i \Delta\theta_2^{\pm}.$$

The solutions to the above optimization problems give rise to the square point shown in Figure 4. Note that these problems correspond to the vertex enumeration subproblems (Swaney and Grossmann, 1985a) proposed to evaluate the flexibility index. Consequently, at this step, one can utilize the results to evaluate the flexibility index that corresponds to the minimum of the results (δ^i), where i denotes different vertices. For this example, it is found that $F = 0.278$ limited by the flexibility point, as shown in Figure 4.

Step 2. Solve the problems of maximizing the deviations from the nominal point by varying one uncertain parameter at a time. The optimization problems solved at this step have the following form

$$\max \delta$$
$$\text{s.t. } f_j(d, z, \theta_1, \theta_2) \le 0, \; j = 1, \ldots, 6$$
$$\theta_1 = \theta_1^N \pm \delta\Delta\theta_1^{\pm}$$
$$\theta_2 = \theta_2^N$$

and

$$\max \delta$$
$$\text{s.t.}$$
$$f_j(d, z, \theta_1, \theta_2) \le 0, \; j = 1, \ldots, 6$$
$$\theta_1 = \theta_1^N$$
$$\theta_2 = \theta_2^N \pm \delta\Delta\theta_2^{\pm}.$$

In this way the points illustrated with the circles in Figure 5 are determined.

Step 3. Quickhull algorithm is applied to identify the convex hull based on the points obtained from steps 1 and 2. The output of the algorithm is the set of linear constraints describing the convex hull. The constraints are given and illus-

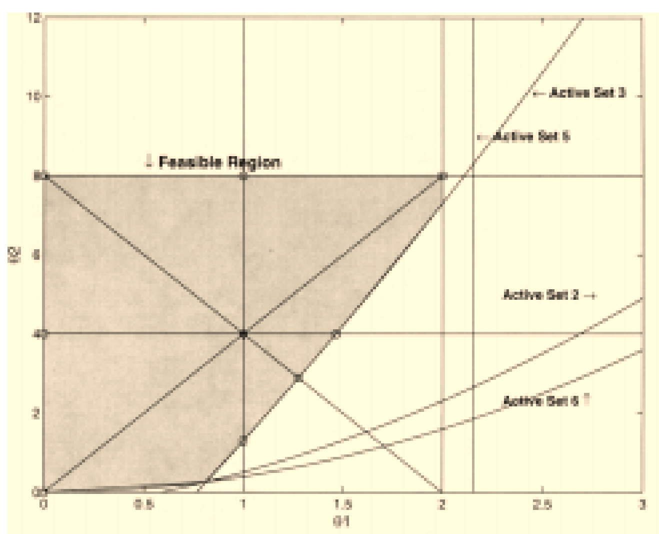

Figure 5. Step 2: Finding points at the boundary (varying one parameter at a time).

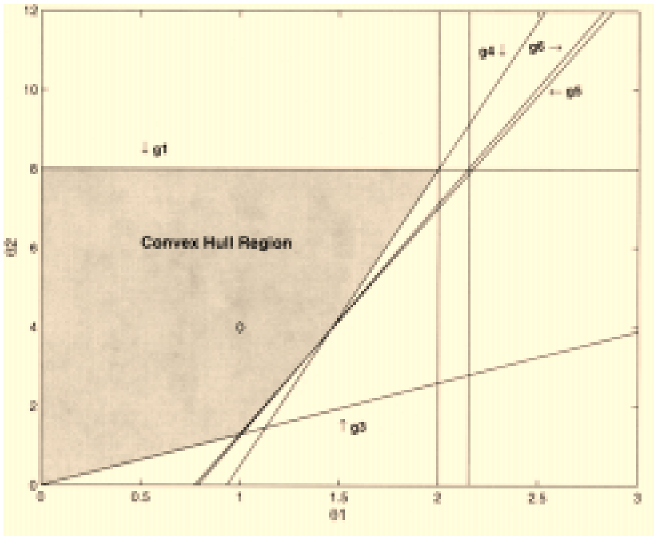

Figure 6. Step 3: Determine the feasible convex hull.

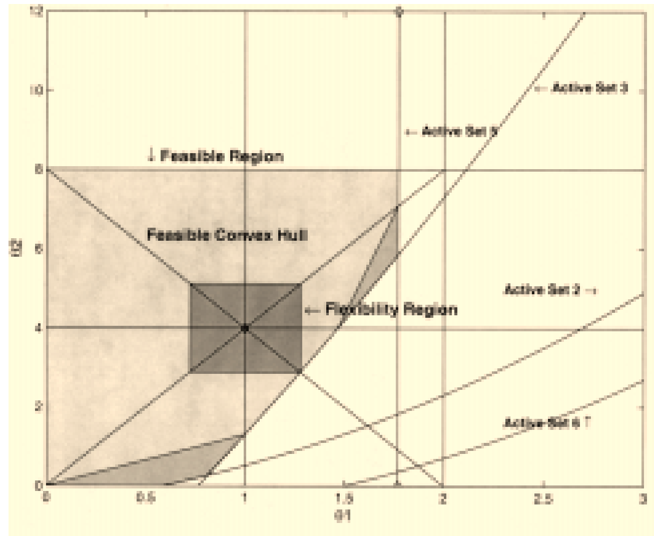

Figure 7. Design 2: Determination of feasible convex hull.

trated in Figure 6

$$g_1 = \theta_2 - 8 \le 0$$

$$g_2 = -\theta_1 \le 0$$

$$g_3 = \theta_2 - 1.3 \times \theta_1 \le 0$$

$$g_4 = \theta_2 - 7.5 \times \theta_1 + 7.0 \le 0$$

$$g_5 = \theta_2 - 5.71 \times \theta_1 + 4.4 \le 0$$

$$g_6 = \theta_2 - 5.88 \times \theta_1 + 4.63 \le 0$$

Step 4. The volume (area in this case, since the problem involves two uncertain parameters) is evaluated at this step using the *Quickhull algorithm* that utilizes *Delaunay Triangulation* to determine the volume of the convex hull. The volume of the overall expected range is also calculated. For this example, it is found that the total volume is 16 units whereas the feasible convex hull has a volume of 10.9 units. This results in a ratio of 0.68 that corresponds to the percentage of design feasibility.

The same procedure is applied for Design 2 ($d_1 = 2.5$, $d_2 = 3.5$). As pointed out in the previous section, the flexibility index for this design has the same value as the flexibility for Design 1 equals to F = 0.278. This is due to the fact that the limiting active set is the same in both cases. However, as shown in Figure 7, Design 2 has a smaller feasible region than Design 1. This is correctly identified by the proposed approach which determines a ratio of feasibility equal to 0.64 for Design 2 compared to 0.68 for Design 1. It is important to point out that the convex hull offers a very accurate description of the feasible region for both designs.

Remark 1. It should be pointed out that the proposed ratio (FCHR) as defined by Eq. 7 corresponds to the percentage of feasibility based on the overall expected range of uncertainty and *not* the true feasibility region. As can be observed from Figures 6 and 7, the percentage that corresponds to the feasible convex hull is much higher in terms of the actual feasible region.

Remark 2. It should be also noted that the proposed methodology for feasible region evaluation and the proposed feasibility metric is not a probabilistic measure and thus does not take into account the probability of uncertainty realizations. Extensions of the proposed work along the lines proposed by Straub and Grossmann (1993) and Pistikopoulos and Mazzuchi (1990) is a subject of present research.

Remark 3. The computational requirements of the proposed approach involve the solution of 2^n optimization problems at step 1, and $2 \times n$ optimization problems at step 2, where n is the number of uncertain parameters involved. However, it should be noted that one can choose to consider a subset of these problems, identify the corresponding points at the boundary of the feasible region and proceed in the next step of evaluating the convex hull.

Examples

Example 1

The first example considered in this section also involves a set of convex constraints that restrict the feasible region

$$f_1 = \theta_2 + \theta_1^2 - \theta_1 - 40 \le 0$$

$$f_2 = \theta_1^2 + \theta_1 - \theta_2 - 2 \le 0$$

$$f_3 = \theta_2 - 4 \times \theta_1 - 30 \le 0$$

The feasible region is shown shaded in Figure 8. We assume that the nominal point is $(\theta_1, \theta_2) = (2.5, 20)$ with expected deviations of $\Delta\theta_1^- = 7.5$, $\Delta\theta_1^+ = 2.5$, $\Delta\theta_2^+ = 20$ and $\Delta\theta_2^- = 60$.

The steps of the proposed analysis are then applied to determine first the points at the boundary of the feasible region and then the feasible convex hull. At step 2 of the procedure, the flexibility index is also evaluated to be equal to F = 0.174. The resulting feasible convex hull has a total volume of 148.7 units, while the expected region corresponds to a volume of

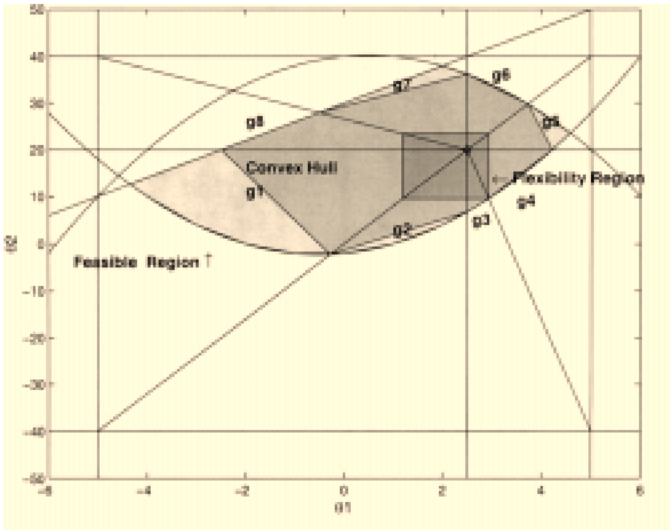

Figure 8. Example 1: feasible convex hull.

800 units, that results in a feasible ratio of FCHR = 0.19. Note that the inscribed convex hull describes the feasible region much more accurately than the flexibility index that corresponds to only 3% of the expected range of variability compared to 19% of the feasible convex hull, as shown in Figure 8. Note that the percentage in terms of the actual feasible region is much higher since only the light shaded areas (Figure 8) are excluded from the feasible convex hull. The value of FCHR is, however, still small because it reflects the ratio of the feasible convex hull region when compared not to the actual feasible region that is unknown, but the expected range of uncertainty which can be much larger.

The exact linear constraints describing the convex hull are

$$g_1 = \theta_2 + 9.98 \times \theta_1 + 4.94 = 0.0$$

$$g_2 = \theta_2 - 3.22 \times \theta_1 + 1.31 = 0.0$$

$$g_3 = \theta_2 - 4.0 \times \theta_1 - 30.0 = 0.0$$

$$g_4 = \theta_2 - 2.75 \times \theta_1 - 29.38 = 0.0$$

$$g_5 = \theta_2 + 20.1 \times \theta_1 - 104.74 = 0.0$$

$$g_6 = \theta_2 + 5.23 \times \theta_1 - 49.32 = 0.0$$

$$g_7 = \theta_2 - 8.4 \times \theta_1 + 15.42 = 0.0$$

$$g_8 = \theta_2 - 5.92 \times \theta_1 + 8.06 = 0.0$$

Example 2

The second example corresponds to the pump and pipe example described by Swaney and Grossmann (1985a). The set of constraints represent the energy balance, the outlet pressure tolerance, the pump driver power limit, and the constraint valve range. By eliminating the outlet pressure P_2 using the energy balance, the reduced set of inequalities is the following

$$f_1 = P_1 + \rho \times H - \frac{m^2}{\rho \times c_v^2} - k \times m^{1.84} \times D^{-5.16} - P_2^* - \epsilon \le 0.0$$

$$f_2 = -P_1 - \rho \times H + \frac{m^2}{\rho \times c_v^2} + k \times m^{1.84} \times D^{-5.16} + P_2^* - \epsilon \le 0.0$$

$$f_3 = m \times H - \eta \times \hat{W} \le 0.0$$

$$f_4 = c_v - c_v^{\max} \le 0.0$$

$$f_5 = -c_v + r \times c_v^{\max} \le 0.0.$$

The design variables are the driver power $\hat{W}$, the pump head H, the pipe diameter D, and the control valve size $c_v^{\max}$, the control variable is the valve coefficient c_v, and the uncertain parameters are the desired pressure $\theta_1 = P_2^*$, and the flow rate $\theta_2 = m$. The expected deviations considered in this example are

$$\Delta\theta_1^+ = 2, \quad \Delta\theta_1^- = 6, \quad \Delta\theta_2^+ = 200, \quad \Delta\theta_2^- = 550.$$

Two designs are examined and evaluated in terms of their feasibility Design 1 that corresponds to the following set of design variables

$$\hat{W} = 31.2, \quad H = 1.3, \quad D = 0.0762, \quad c_v^{\max} = 0.0577$$

and Design 2 that corresponds to the following design values,

$$\hat{W} = 33.74, \quad H = 1.406, \quad D = 0.0764, \quad c_v^{\max} = 0.093408.$$

The proposed approach is applied to both designs in order to evaluate the feasible convex hull. Figures 9 and 10 show the results.

It is found that the feasibility ratio is FCHR = 0.97 for design 1 and 0.92 for design 2 compared to flexibility index that

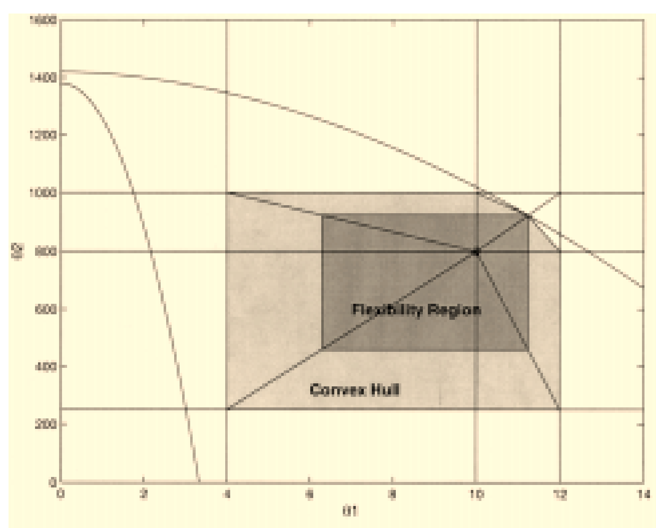

Figure 9. Example 2: feasible convex hull for design 1.

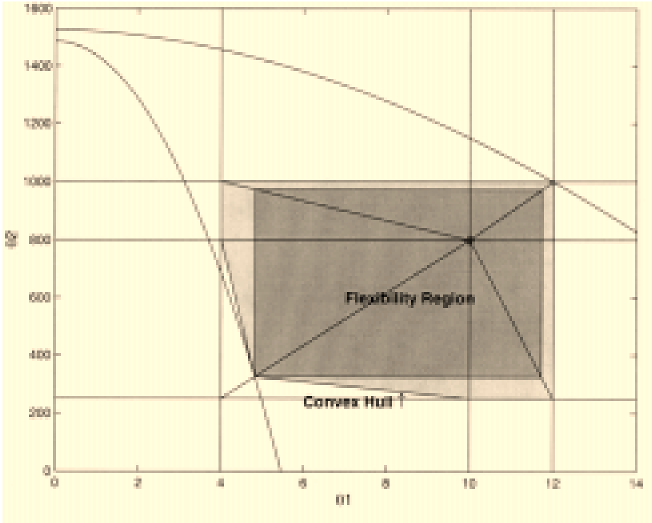

Figure 10. Example 2: feasible convex hull for design 2.

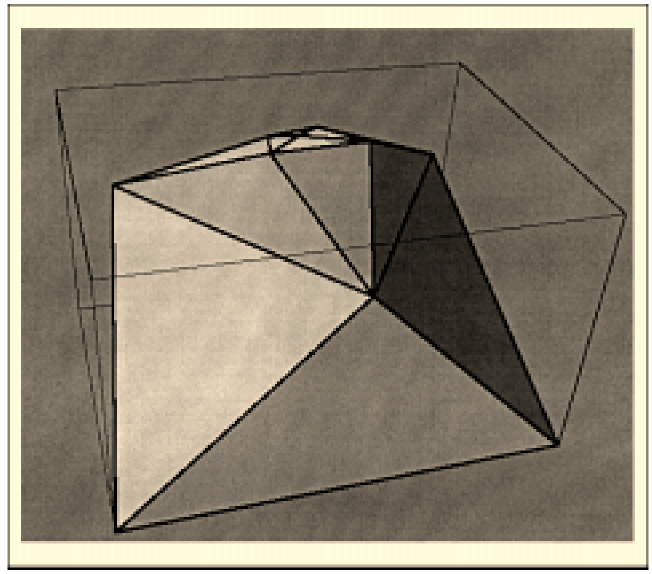

Figure 11. Example 3: feasible convex hull for 3-D feasible region.

is 0.618 for design 1 and 0.863 for design 2. Consequently, by evaluating the feasible convex hull, we can better compare the feasibility of different designs since, as shown in Figures 9 and 10, design 1 has actually larger feasible region than design 2 which could not be captured by the flexibility index. The major advantage of the proposed approach compared to the flexibility index is that it is not limited by one direction, but can capture the overall design behavior under parameter variability. However, it should be pointed out that since the feasible region is 1-DQC and not jointly convex on θ_1, θ_2, there is no guarantee that the convex hull defined by the points found through steps 1 and 2 would be inscribed within the feasible region. To overcome this difficulty the approach described in the following section is modified as suggested.

Example 3

The example considered here is a modification of the example of Pistikopoulos and Ierapetritou (1995) with three uncertain parameters. The constraints described the feasible region of the design (d_1, d_2) have the following form

$$f_1 = -z - \theta_1 + 0.5\times\theta_2^2 + 2.0\times\theta_3^2 + d_1 - 3\times d_2 - 8 \le 0$$

$$f_2 = -z - \theta_1/3 - \theta_2 - \theta_3/3 + d_2 + 8/3 \le 0$$

$$f_3 = z + \theta_1\times\theta_1 - \theta_2 - d_1 + \theta_3 - 4 \le 0$$

where z is the control variable, $\theta_1, \theta_2, \theta_3$ are the uncertain parameters with nominal value of $\theta_1^N = \theta_2^N = \theta_3^N = 2$ and expected deviations $\Delta\theta_1^{\pm} = \Delta\theta_1^{\pm} = \Delta\theta_1^{\pm} = 2$. All the constraints are jointly convex on (θ) and (z). The design examined here corresponds to $(d_1,\ d_2) = (3,1)$. The proposed approach is applied for this design and the following points are first identified at the boundary of the feasible region.

Step 1. At the first step, the points towards the vertices of the expected uncertainty range:

$$\text{p1: } (\theta_1, \theta_2, \theta_3) = (2.218,\ 2.218,\ 2.218)$$
$$\text{p2: } (\theta_1, \theta_2, \theta_3) = (3.000,\ 3.000,\ 1.000)$$
$$\text{p3: } (\theta_1, \theta_2, \theta_3) = (2.252,\ 1.748,\ 2.252)$$
$$\text{p4: } (\theta_1, \theta_2, \theta_3) = (1.637,\ 2.363,\ 2.363)$$
$$\text{p5: } (\theta_1, \theta_2, \theta_3) = (2.486,\ 1.514,\ 1.514)$$
$$\text{p6: } (\theta_1, \theta_2, \theta_3) = (1.514,\ 1.514,\ 2.455)$$
$$\text{p7: } (\theta_1, \theta_2, \theta_3) = (0.000,\ 4.000,\ 0.000)$$
$$\text{p8: } (\theta_1, \theta_2, \theta_3) = (0.000,\ 0.000,\ 0.000).$$

Step 2. Varying only one uncertain parameter at the time we got the following points:

$$\text{p9: } (\theta_1, \theta_2, \theta_3) = (2.622,\ 2.000,\ 2.000)$$
$$\text{p10: } (\theta_1, \theta_2, \theta_3) = (0.000,\ 2.000,\ 2.000)$$
$$\text{p11: } (\theta_1, \theta_2, \theta_3) = (2.000,\ 2.000,\ 2.312)$$
$$\text{p12: } (\theta_1, \theta_2, \theta_3) = (2.000,\ 2.000,\ 0.000)$$
$$\text{p13: } (\theta_1, \theta_2, \theta_3) = (2.000,\ 3.646,\ 2.000)$$
$$\text{p14: } (\theta_1, \theta_2, \theta_3) = (2.000,\ 0.667,\ 2.000).$$

Step 3. Then the quickhull algorithm is applied to determine the feasible convex hull of the points obtained at steps 1 and 2. The resulting convex hull is illustrated in Figure 11.

Step 4. Using *Delaunay Triangulation* the volume of the convex hull is determined to be equal to 12.26 that corresponds to 19% of the total expected range of uncertainty.

To compare with the results of the flexibility analysis the flexibility of the design is also determined F = 0.109. The volume of the corresponding rectangular is approximately 0.083 that corresponds to only 0.12% of the expected uncertainty range (see Figure 12).

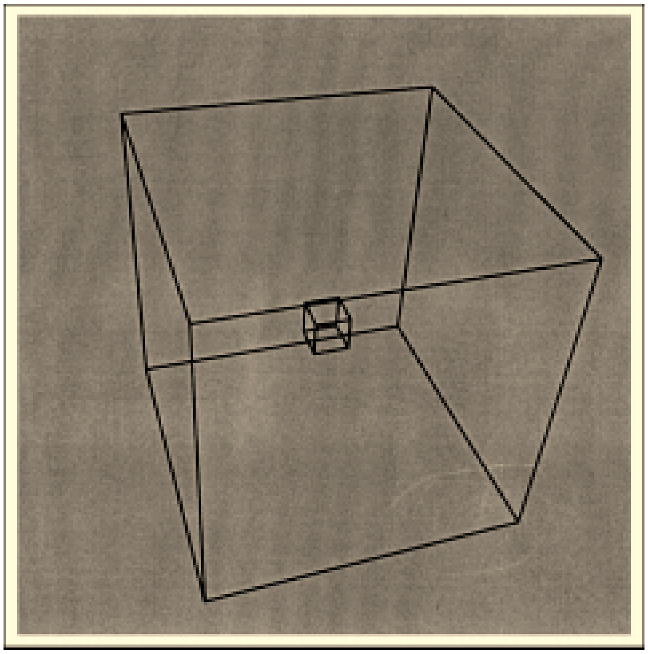

Figure 12. Example 3: Flexibility range and overall expected range of uncertainty.

1DQC Convex Feasible Region

First, it should be pointed out that only 1-D convex regions are examined here and not general nonconvex regions which is the subject of the second part of this work. For the case of the 1-D convex region, the proposed approach is similar to the approach for the convex case with the difference that after evaluating the points at the boundary towards the vertices as described at step 1, the nonconvex constraints are linearized at these points. It should be noted that only the nonconvex constraints that are active at these points are linearized and not all of the nonlinear constraints in the problem. Since then constraints considered here are jointly quasi-convex in z and 1-D quasi-convex in (θ), it is proven that the linearization would always result in underestimation of the feasible region (see Appendix A). In the following section an example involving 1-D quasi-convex functions is considered to illustrate the results of the proposed approach for this case.

Example 4

The example presented in this section corresponds to an example that exhibits a 1-D convex feasible region. To illustrate the proposed ideas, the example is simple and described by the following constraints

$$f_1 = -\theta_2 + \theta_1 \times \theta_1 + 2 \times \theta_1 \leq 0$$

$$f_2 = \theta_2 \times (6 + \theta_1) - 350 \leq 0$$

$$f_3 = \theta_2 + \theta_1 \times \theta_1 - 60 \leq 0$$

$$f_4 = \theta_2 - 10 \times \theta_1 - 50 \leq 0.$$

Note that the constraints satisfy properties (2) and (3) proved by Swaney and Grossmann (1985a) to be sufficient in resulting in the 1DQC feasible region (as also shown in Figure 13.)

The proposed approach is applied for this example and the feasible convex hull is determined (Figure 13). Note that, for comparison purposes, the approach is applied for both the original nonconvex constraints, as well as the convexified ones. As suggested in the previous section, the convexification is obtained after the determination of the points at the boundary. For this example, the point used to convexify the nonconvex constraint f_2 is the point (P1) shown in Figure 14 identified from the optimization problem of maximizing the deviation from the nominal point towards the vertex that corresponds to the maximum positive deviations of θ_1, θ_2. The convexification results in the following linear constraint shown in Figure 14 with a dashed line

$$\hat{f}_2 = \theta_2 - 51.385 + 4.17 \times \theta_1 \leq 0.0$$

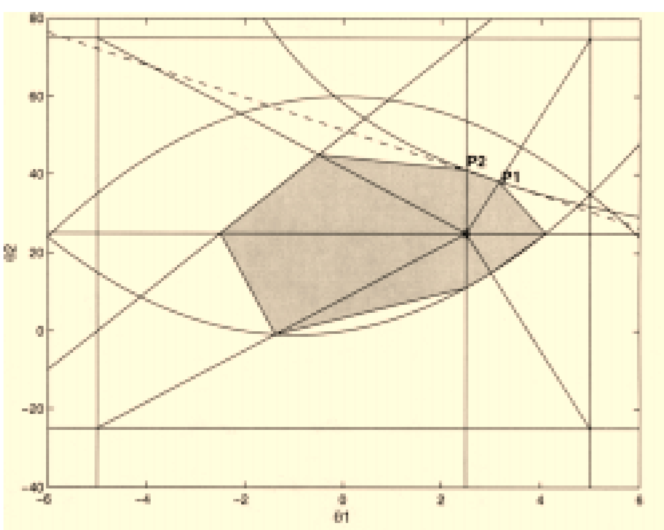

Figure 13. Example 4: feasibility convex hull for 1DQC feasible region.

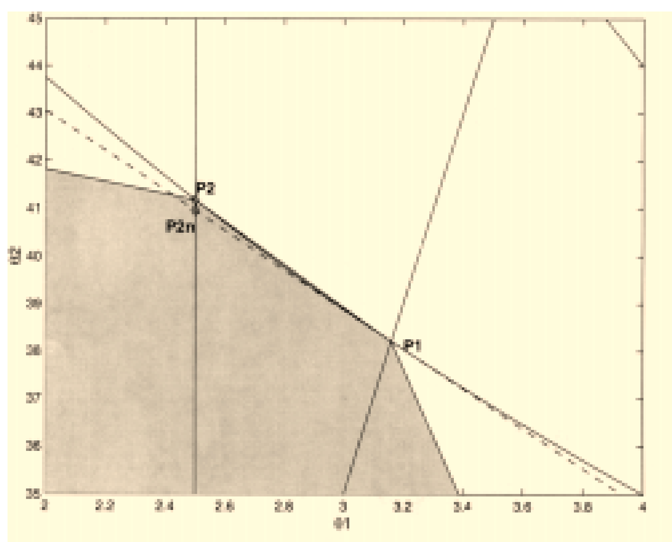

Figure 14. Example 4: convexification of constraint f_2.

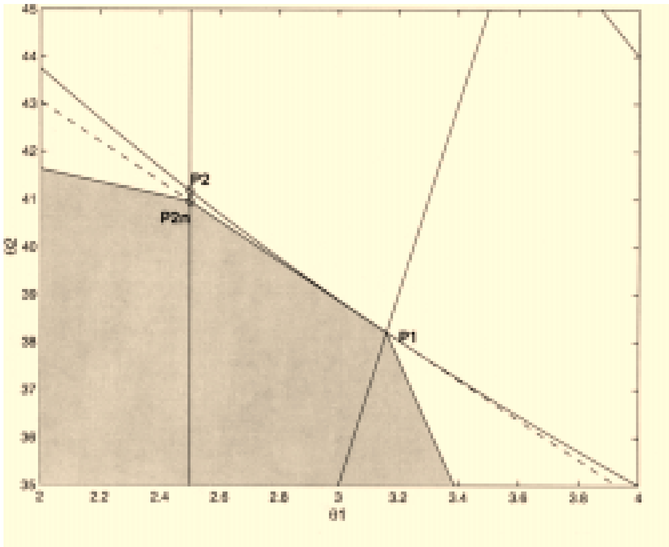

Figure 15. Example 4: feasible convex hull for 1DQC feasible region using convexified constraint.

Using this constraint instead of constraint f_2 results in the determination of point (P2n) to be used on feasible convex hull evaluation instead of point P_2 (Figure 14).

Since the difference is very small in this example, we illustrate the result by focusing Figure 15 at the area of point (P2) which is the only difference between the feasible convex hull of the original problem and the feasible convex hull of the convexified problem.

Discussion and Future Directions

A novel approach for evaluating the range of feasibility of a given process is proposed in this article. The basic idea is to determine the convex hull that can be inscribed within the feasible region. The convex hulls were computed using the *Quickhull Algorithm* which is an incremental algorithm for evaluating the convex hull given a set of points. The points used to determine the feasible convex hull are points at the boundary of the feasible region that are obtained from the solution of a series of small optimization subproblems. The outcome of the application of the *Quickhull Algorithm* is not only the computation of the convex hull described by a set of linear constraints but also its volume. This is achieved based on the ideas of *Delaunay Triangulation*. A new metric was introduced that corresponds to the ratio of the feasible convex hull volume divided by the overall expected range of uncertainty. In all examples considered we found that the proposed approach results in much better description of the feasible space. Moreover, the new metric introduced to represent the feasibility of a given process was found to describe accurately the feasible space and thus results in correct comparison between different designs and/or processes.

Although the examples addressed in this work are of small scale, the results obtained are very promising regarding the applicability of the proposed work in large-scale problems. Different extensions are currently under investigation regarding (a) the applicability of the work to nonconvex case, and (b) the development of efficient implementation scheme exploiting the inherent distributed nature of the initial steps of the proposed approach, and (c) the extension of the proposed work to incorporate the probability of occurrence of uncertain parameter realizations.

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Appendix: Proof of Feasible Region Underestimation

Proposition

If $f_j(d, z, \theta)$ are jointly quasi-convex in z and 1-D quasi-convex in θ, then the linearization around and extreme point underestimates the feasible region.

Proof

As illustrated in Figure A1, we need to basically to prove that the point θ^1 belongs in the feasible region, that is,

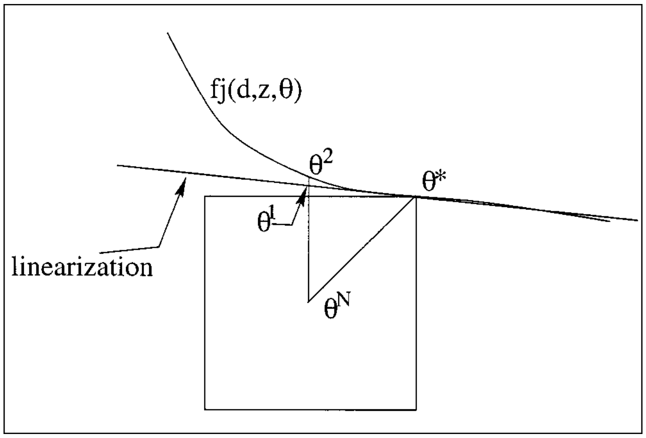

Figure A1. Underestimation of feasible region.

$\psi(d,\theta^1) \le 0$. Since θ^* and θ^2 are at the boundary $\psi(d,\theta^*) = \psi(d,\theta^2) = 0$ as proved by Swaney and Grossmann (1985a). Also, we assume that the nominal point is a feasible point and thus $\psi(d,\theta^N) \le 0$. Since θ^1 belongs to the line with slope $\nabla f_j(d,z,\theta)(\theta^*)$ there exist a scalar α such that $\theta^1 = \alpha\theta^N + (1-\alpha)\theta^2$. Based on theorem proved by Swaney and Grossmann (1985a), if the constraint functions $f_j(d,z,\theta)$ are jointly quasi-convex in z and one-dimensional quasi-convex in θ, then the feasibility function $\psi(d,\theta)$ is 1-D quasi-convex in θ,

$$\psi(d,\theta^1) \le \max\{\psi(d,\theta^2), \psi(d,\theta^N)\}.$$

Since $max\{\psi(d,\theta^2),\ \psi(d,\theta^N)\} = 0$, $\psi(d,\theta^1) \le 0$ and the proposition has been proved.

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