

Identification of Vertex and Nonvertex Critical Points for Large-Scale Approximate Stochastic Optimization

Zorka Novak Pintarič, Zdravko Kravanja

University of Maribor, Faculty of Chemistry and Chemical Engineering
Smetanova 17, SI 2000 Maribor, Slovenia

Abstract

This paper presents a strategy for optimal design of chemical processes with stochastic uncertain parameters defined inside bounded intervals. Strategy relies on approximate stochastic optimization at one single point, called the central basic point (CBP), while desired flexibility is achieved by simultaneous consideration of critical points. The CBP method has been extensively described elsewhere (Novak Pintarič and Kravanja, 2004). The aim of this work is to develop a procedure for determining a minimal set of critical points, which can identify vertex and nonvertex critical points. In this procedure the uncertain parameters are transformed into continuous variables, and a special NLP problem is solved for each design variable in order to determine the most unfavourable combination of uncertain parameters which would force a given design variable to its maximum. The procedure avoids explicit enumeration of all vertices and is thus suitable for solving problems with several tens of uncertain parameters. Two examples are presented of heat exchanger network design with vertex and nonvertex critical points.

Keywords: flexibility, design, nonvertex critical points

1. Introduction

The problem of process design under uncertainty involves two main challenges: first, accurate determination of the expected objective function and, second, the generation of a design which is flexible over the whole region of uncertainty. Both problems are concerned with highly discretized models and heavy computing requirements. For the first task various integration schemes have been proposed (e.g. Acevedo and Pistikopoulos, 1998) and recently, approaches for reducing the computational effort, e.g. a cubature technique by Bernardo et al. (1999), and the central basic point (CBP) method for approximate stochastic optimization by Novak Pintarič and Kravanja (2004). The second task is connected with the detection of a minimal set of points required to achieve flexible design. Halemane and Grossmann (1981) showed that in convex problems these points correspond to the extreme vertices and proposed an iterative multi-period design algorithm in which the set of critical vertices is determined based on the procedure suggested by Grossmann and Sargent (1978). However, in nonconvex problems, critical points may lie inside the intervals of uncertain parameters.

In this work we present a strategy for the approximate stochastic optimization of problems with bounded uncertain parameters. Strategy consists of three steps: 1) identification of critical points, 2) determination of central basic point (CBP) and 3) simultaneous optimization of a model at CBP and critical points. The last two steps are described in our previous work (Novak Pintarič and Kravanja, 2004), while in this work we present a procedure for identifying a minimal set of vertex and nonvertex critical points. The term critical points used in this work is related to the points that are critical for determining the optimal overdesign of process units and, thus, determining the flexibility of the solution.

2. A strategy for approximate stochastic optimization

Mathematical model for optimization under uncertainty is in general an infinite program that is usually solved by discretization of the uncertain space over points $\theta_k, k=1,2,\dots,n_p$:

<i>Infinite model :</i> $\min_{x,d} C(x,d,\theta)$ s.t. $h(x,d,\theta) = 0 \quad (1)$ $g(x,d,\theta) \leq 0$ $d \geq g_d(x,\theta)$ $x \in X, d \in D, \theta \in TH$	$\xrightarrow{\text{Discretization}}$	<i>Discretized model :</i> $\min_{x_k,d} EC(x_k,d,\theta_k)$ s.t. $h_k(x_k,d,\theta_k) = 0 \quad (2)$ $g_k(x_k,d,\theta_k) \leq 0 \quad k = 1,2,\dots,n_p$ $d \geq g_{d,k}(x_k,\theta_k)$ $x_k \in X, d \in D, \theta_k \in TH$
---	---------------------------------------	---

where EC represents the expected value of the objective function C , x is the vector of state and control variables, d is the vector of design variables and θ is the vector of uncertain parameters. h , g and g_d represent equality, inequality and design inequality constraints, respectively. Accurate solution of a discretized problem may require an extensive set of points. In the proposed strategy, the number of discretized points is reduced significantly as the expected value is approximated at one single point (CBP) while the desired flexibility is assured with a minimal set of critical points determined in the following procedure.

2.1 Identification of vertex and nonvertex critical

In this paper, critical point defines a combination of uncertain parameters for which a given problem requires maximal overdesign to achieve desired flexibility. In order to determine critical points, a problem for maximization of the design variable under study, $d_i, i=1,2,\dots, n_d$, is formulated in which uncertain parameters are the only degrees of freedom. Suppose that uncertain parameters in the infinite model (1) are transformed into continuous variables. Then, by applying the underlying first order Karush-Kuhn-Tucker (KKT) optimality conditions with respect to x and d , a system of equations is obtained with θ being the only degrees of freedom. However, since applying KKT conditions explicitly to large and complex problems is impractical, an alternative method is to use the following bilevel problem where in every iteration maximization of d_i is performed at the upper level, while at the lower level, the cost minimization problem (1) is solved for current values of θ :

$$\begin{aligned}
& \max_{\theta} d_i \\
& \text{s.t.} \quad d_i = f(\min_{x,d} C(x,d,\theta)) \quad \forall i = 1, 2, \dots, n_d \\
& \quad x, d \in R \\
& \quad \theta = \{\theta_j, \theta_j^{\text{LO}} \leq \theta_j \leq \theta_j^{\text{UP}}\} \in TH \subset R, j = 1, 2, \dots, n_u
\end{aligned} \tag{3}$$

Investigation and computer implementation of the above formulation is under way. So far the following approximate one-level nonlinear programming problem (NLP)_i has been implemented:

$$\begin{aligned}
& \min_{x,d,\theta} C(x,d,\theta) - M \cdot d_i \\
& \text{s.t.} \quad h(x,d,\theta) = 0 \\
& \quad g(x,d,\theta) \leq 0 \\
& \quad d = g_d(x,\theta) \\
& \quad x, d \in R \\
& \quad \theta = \{\theta_j, \theta_j^{\text{LO}} \leq \theta_j \leq \theta_j^{\text{UP}}\} \in TH \subset R, j = 1, 2, \dots, n_u
\end{aligned} \tag{NLP}_i$$

$i=1, 2, \dots, n_d$

Note that in problem (NLP)_i design variable d_i is forced to its maximum by subtracting d_i multiplied by a large scalar M , from the cost function C . In this way higher priority is given to the maximization of d_i than to the minimization of cost C .

The result of this step is a matrix, t_{ij} , $i=1, 2, \dots, n_d$, $j=1, 2, \dots, n_u$, where t_{ij} is either the vertex or nonvertex value of uncertain parameter θ_j obtained when solving problem (NLP)_i for maximization of design variable d_i . The influence of uncertain parameters on design variables is analyzed by formulating the matrix of derivatives, m_{ij} , which can be numerically obtained as ratios of the marginal values of d_i with respect to the marginal values of θ_j . Derivatives are compared inside each θ_j column and their relative absolute values are calculated:

$$r(d_i, \theta_j) = \frac{|m_{ij}|}{\max_i |m_{ij}|} \quad \text{where} \quad m_{ij} = \left[\frac{\partial d_i}{\partial \theta_j} \right] \tag{4}$$

$j = 1, 2, \dots, n_u \quad i = 1, 2, \dots, n_d, \quad j = 1, 2, \dots, n_u$

If $r(d_i, \theta_j) > \varepsilon$, where ε is a small constant, e.g. 10^{-6} , uncertain parameter θ_j influences design variable d_i and corresponding value t_{ij} is considered for merging with other components into the final reduced set of critical points, so that all combinations of influential uncertain parameters are retained. The merging procedure is straightforward for small examples, while for larger examples a more systematic approach must be applied, e.g. set covering formulation (Grossmann and Sargent, 1978).

The attractive feature of the proposed procedure is that the maximal number of critical points, n_c , is equal, or less than, the number of design variables. Another advantage is that the proposed (NLP)_i problem is not discretized and, therefore, the size of the model is similar to the one of the original deterministic problem. Moreover, explicit enumeration of all vertices is avoided and, as stated, KKT conditions need not be derived explicitly, which is especially favourable for large models with complex constraints.

2.2 Determination of CBP

When critical points are identified, the next step is the determination of the central basic point (see Novak Pintarič and Kravanja, 2004), which provides good approximation of the expected objective function. CBP is determined through a one-dimensional integration problem, where the conditional expected value is calculated for each uncertain parameter. These problems are solved over the set of critical points and quadrature points (usually 5) of uncertain parameter under study giving the maximum number of discrete points to be n_c+5 . Based on the values obtained, regression is used for every uncertain parameter to determine its value for which the objective function equals the conditional expected value. These values represent the components of the CBP. The lower bounds of the design variables are also determined during the set-up procedure.

2.3 Approximate stochastic optimization

Approximate stochastic optimization is finally performed at the CBP, θ^{CBP} , and critical points, θ_k^c , $k=1,2,\dots,n_c$ yielding a model discretized at n_c+1 points where n_c is usually less than the number of design variables, n_d :

$$\begin{aligned} \min_{x,d} C(x,d,\theta^{\text{CBP}}) \\ \text{s.t.} \quad & \left. \begin{aligned} h(x,d,\theta^{\text{CBP}}) &= 0 & h_k(x_k,d,\theta_k^c) &= 0 \\ g(x,d,\theta^{\text{CBP}}) &\leq 0 & g_k(x_k,d,\theta_k^c) &\leq 0 \\ d &\geq g_d(x,\theta^{\text{CBP}}) & d &\geq g_{d,k}(x_k,\theta_k^c) \end{aligned} \right\} k=1,\dots,n_c \quad (\text{NLP-AF}) \\ & d \geq d^{\text{LO}}; x, x_k, d \in R \end{aligned}$$

3. Example with vertex critical point

This example considers a small heat exchanger network (Fig.1) with a fixed structure.

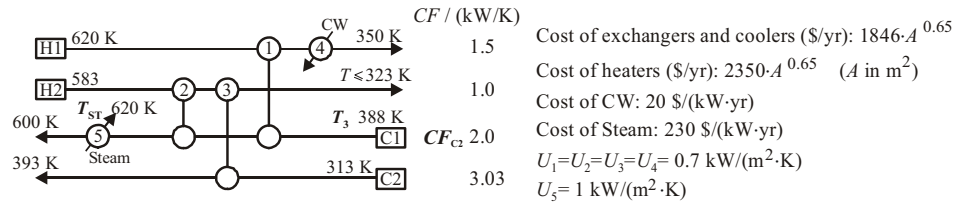


Figure 1: Heat exchanger network example

Four uncertain parameters are distributed normally by the following means, θ^i , and standard deviations, σ : T_3 , $N[388, 3.33]$ K; U_1 , $N[0.7, 0.0466]$ kW/(m²·K); CF_{C1} , $N[2, 0.066]$ kW/K and T_{ST} , $N[620, 5]$ K. The bounds are determined to be $\theta^i \pm 3\sigma$. The mathematical model includes the equations for heat balances, constraints on temperature differences and design correlations for the heat transfer areas of five exchanger units. The total cost is minimized and composed of operating and annualized investment costs.

a) *Identification of critical points.* In the first step, problems (NLP)_i, $i=1,2,\dots,5$, are solved for five areas giving the results in Table 1. Note that uncertain parameters obtain the extreme values solely.

Table 1: Determination of vertex critical points

Values of uncertain parameters, t_{ij}					Relative derivatives ($\varepsilon=10^{-6}$)			
max	T_3	U_1	CF_{C2}	T_{ST}	$r(A_i/T_3)$	$r(A_i/U_1)$	$r(A_i/CF_{C2})$	$r(A_i/T_{ST})$
A_1	<u>398</u> ^{UP}	<u>0.56</u> ^{LO}	<u>2.2</u> ^{UP}	<u>635</u> ^{UP}	1	1	1	$<\varepsilon$
A_2	<u>378</u> ^{LO}	<u>0.84</u> ^{UP}	<u>1.8</u> ^{LO}	<u>635</u> ^{UP}	$<\varepsilon$	$<\varepsilon$	0.14	$<\varepsilon$
A_3	<u>378</u> ^{LO}	<u>0.84</u> ^{UP}	<u>1.8</u> ^{LO}	<u>635</u> ^{UP}	$<\varepsilon$	$<\varepsilon$	$<\varepsilon$	$<\varepsilon$
A_4	<u>398</u> ^{UP}	<u>0.84</u> ^{UP}	<u>1.8</u> ^{LO}	<u>635</u> ^{UP}	10^{-4}	$<\varepsilon$	10^{-5}	$<\varepsilon$
A_5	<u>378</u> ^{LO}	<u>0.84</u> ^{UP}	<u>2.2</u> ^{UP}	<u>605</u> ^{LO}	0.6	$<\varepsilon$	0.16	1

Relative derivatives larger than ε (assumed to be 10^{-6}) determine values, t_{ij} , that contribute to the formation of critical points. In this example the underlined values in Table 1 define three critical points for $(T_3, U_1, CF_{C2}, T_{ST})$: $\theta_1^C = (398, 0.56, 2.2, 605)$, $\theta_2^C = (398, 0.56, 1.8, 605)$ and $\theta_3^C = (378, 0.56, 2.2, 605)$.

b) *Determination of CBP*. The set-up procedure as described elsewhere, gives the following CBP: $\theta^{CBP} = (387.309, 0.692, 2.006, 620)$ and the lower bounds on the design variables are $A^{LO} = (15.29, 2.13, 6.14, 2.26, 5.63) \text{ m}^2$.

c) *Solution of approximate flexibility problem (NLP-AF)*. Finally, the problem was solved at the CBP and three critical points with the lower bounds on design variables giving an expected cost of 48 735 \$/yr and $A = (15.77, 2.13, 6.15, 2.26, 5.63) \text{ m}^2$. The flexibility index of this design, determined through 16 vertex points, is equal to or greater than 1 which indicates that the design obtained has exactly the desired flexibility for feasible operation over defined intervals of uncertain parameters. The stochastic optimization of this example was also performed with rigorous Gaussian integration simultaneously at $5^4=625$ quadrature points and 16 vertex points, giving a flexible solution with the expected cost of 49 111 \$/yr and $A = (14.71, 2.26, 6.33, 2.23, 5.62) \text{ m}^2$. Good agreement of the approximate CBP method with more rigorous one is established.

4. Example with nonvertex critical point

A similar problem as before was studied. A new uncertain parameter θ_F , $N[1, 0.06666]$, was introduced with additional constraint, $A_1 = -146 \cdot \theta_F^2 + 334 \cdot \theta_F - 158$, which imposes a maximum value of A_1 inside the interval $[0.8, 1.2]$ at $\theta_F = 1.144$. Other uncertain parameters are T_3 , $N[388, 3.33] \text{ K}$; U_2 , $N[0.7, 0.0466] \text{ kW}/(\text{m}^2 \cdot \text{K})$ and T_{ST} , $N[620, 5] \text{ K}$.

a) *Identification of critical points*. The procedure determines two nonvertex values of uncertain parameters: 1.144 for θ_F and 382.2 for T_3 (Table 2). Four critical points are obtained from relative derivatives for $(T_3, \theta_F, U_2, T_{ST})$: $\theta_1^C = (378, 1.144, 0.84, 635)$, $\theta_2^C = (382.2, 1.144, 0.56, 635)$, $\theta_3^C = (398, 1.144, 0.56, 605)$ and $\theta_4^C = (378, 1.144, 0.56, 605)$.

b) *Determination of CBP*. The set-up procedure determines $\theta^{CBP} = (388.64, 1, 0.696, 620)$ and $A^{LO} = (33.02, 4.23, 6.07, 1.69, 4.05) \text{ m}^2$.

c) *Solution of approximate flexibility problem (NLP-AF)*. The problem was solved at the CBP and four critical points with the lower bounds on design variables giving an expected cost of 52 064 \$/yr and $A = A^{LO}$. The flexibility index of this design determined at vertices and at nonvertex point for θ_F is equal to or greater than 1. Stochastic optimization at 625 quadrature points and 16 vertices yields an expected cost of 51 997

\$/yr and design $A = (32.83, 4.18, 6.07, 1.69, 4.05) \text{ m}^2$. The flexibility index of this design is equal to or greater than 1 at vertices, but less than 1 at some nonvertex points, e.g. 0.75 at the point (378, 1.144, 0.56, 635). This indicates that vertex and quadrature points without nonvertex critical points cannot assure the desired flexibility and that the cost function is underestimated.

Table 2: Determination of vertex and nonvertex critical points

max	Values of uncertain parameters, t_{ij}				Relative derivatives ($(\varepsilon=10^{-6})$)			
	T_3	θ_F	U_2	T_{ST}	$r(A_i/T_3)$	$r(A_i/\theta_F)$	$r(A_i/U_2)$	$r(A_i/T_{ST})$
A_1	378^{LO}	1.144	0.84^{UP}	635^{UP}	1	1	1	1
A_2	382.2	0.8^{LO}	0.56^{LO}	635^{UP}	0.09	$<\varepsilon$	0.19	$<\varepsilon$
A_3	378^{LO}	0.8^{LO}	0.84^{UP}	635^{UP}	$<\varepsilon$	$<\varepsilon$	$<\varepsilon$	$<\varepsilon$
A_4	398^{UP}	0.8^{LO}	0.84^{UP}	635^{UP}	0.05	$<\varepsilon$	$<\varepsilon$	$<\varepsilon$
A_5	378^{LO}	0.8^{LO}	0.84^{UP}	605^{LO}	0.03	$<\varepsilon$	$<\varepsilon$	0.31

5. Conclusions

A strategy for the optimal design of problems with stochastic uncertain parameters is presented which significantly reduces the dimensionality of extensive discretized problems. The reduction is achieved with approximation of the expected value at single central basic point which is determined through a one-dimensional set-up procedure. Optimal overdesign is assured at the critical points that can be vertex or nonvertex and are obtained by the solution of special NLP problems with uncertain parameters as degrees of freedom. These problems are only executed for every design variable yielding critical points whose total number is usually less than the number of design variables. The procedure avoids explicit enumeration of all vertices and the derivation of KKT optimality conditions. An investigation is under way to exploit these features for solving complex problems with several tens of uncertain parameters.

References

- Acevedo, J. and E. Pistikopoulos, 1998, Stochastic optimization based algorithms for process synthesis under uncertainty, *Computers and Chemical Engineering* 22, 647.
- Bernardo, F.P., E.N. Pistikopoulos and P.M. Saraiva, Robustness criteria in process design optimization under uncertainty, *Computers and Chemical Engineering* 23, 459.
- Grossmann, I.E. and R.W.H. Sargent, 1978, Optimum design of chemical plants with uncertain parameters, *AIChE Journal* 24, 1021.
- Halemane, K.P. and I.E. Grossmann, 1983, Optimal process design under uncertainty, *AIChE Journal* 29, 425.
- Novak Pintarič, Z. and Z. Kravanja, 2004, A strategy for MINLP synthesis of flexible and operable processes, *Computers and Chemical Engineering* 28, 1105.

Acknowledgements

The authors are grateful for the financial support of Slovenian Ministry of Higher Education, Science and Technology (Program P2-0032 and Project J2-6637).