NONLINEAR ROBUST OPTIMIZATION WITH UNCERTAIN EQUALITY CONSTRAINTS

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Abstract

The problem of nonlinear optimization for process design under uncertainty is addressed in this paper. A novel robust optimization framework is proposed to address general nonlinear problems under uncertainty. To address the limitation of single point linearization with respect to uncertain parameters for a large uncertainty region, an iterative algorithm is developed. The new method applies local linearization around multiple realizations of the uncertainty, and iteratively solves a robust optimization problem. The proposed method can handle uncertainty in both inequality constraints and equality constraints.

Keywords

Nonlinear Programming, Robust Optimization, Process Design

Introduction

Many process design problems can be formulated as nonlinear optimization problems. It is common that uncertain parameters exist in those models since they are often estimated through noisy data. The uncertainty should be considered in optimization, otherwise suboptimal or infeasible solutions may occur.

Robust optimization has become an active research area for handling uncertainty in optimization problems, especially for linear optimization problems (Ben-Tal and Nemirovski, 1999; Bertsimas and Sim, 2004; Li et al., 2011), second-order cone programming (El Ghaoui and Lebret, 1997; Ben-Tal et al., 2002), and semi-definite programming problems (Ben-Tal et al., 1998; El Ghaoui et al., 1998). On the other hand, general nonlinear robust optimization has received less attention in the past. An approximate robust formulation that employs linearization of the model equations at a point corresponding to the nominal parameter values and the chosen values for control variables, the worst-case can be computed through a numerically tractable approximation of the robust counterpart (Diehl et al., 2006). A robust optimization method has been studied based on linearization around nominal values of the uncertain parameters (Zhang, 2007). However, the above methods can only deal with the optimization problem under uncertainty with a small perturbation.

In this paper, a novel nonlinear robust optimization framework is proposed. The objective is to address general nonlinear optimization problems under relatively large uncertainty region. The proposed method is based on linearization with respect to uncertain parameters around multiple realizations and an iterative algorithm. The problems to be addressed can be classified as two categories. In the first case, only inequality constraints are involved with uncertainty. In the second case, both design variables and state variables appear in the nonlinear optimization problem, and they are coupled by the state equations.

The rest of the paper is organized as follows: In the second section, the problem addressed in this paper is formally presented. In the third section, the robust counterpart formulation is derived for both inequality-only case and the general case with equality constraints. In the fourth section, an iterative algorithm is presented, which is based on linearization around multiple realizations of uncertainty. Finally, the proposed method is demonstrated through a process design example.

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Problem Statement

In this work, the following general nonlinear optimization problem for process design is considered:

$$\begin{aligned} \min_{y,u\in U} \quad & \phi(y,u) \\ s.t. \quad & F(y,u,s)=0 \\ & G(y,u,s)\leq 0 \end{aligned} \tag{1}$$

where $s \in R^{N_s}$ represents uncertain parameters, and $y \in R^{N_y}$ represents state variables, $u \in R^{N_u}$ represents design variables which are constrained in a feasible set U, $F(y,u,s)=0$ is known as the state equation. N_s, N_y, and N_u represent the number of the uncertain parameters, state variables, and design variables, respectively.

The size of the state variables y and the number of the state equations F should be equal so that the state variables can be uniquely determined by the design variables and uncertain parameters through the state equations. Based on the Implicit Function Theorem, the state equation $F(y,u,s)=0$ implicitly defines a function $y=y(u,s)$. Throughout the paper, it is assumed that the function F and G are continuously differentiable.

If the state variables y can be eliminated through the state equation, an inequality-only constrained nonlinear optimization can be formulated as follows:

$$\begin{aligned} \min_{u\in U} \quad & \phi(u) \\ s.t. \quad & G(u,s)\leq 0 \end{aligned} \tag{2}$$

where $G=(g_1,...,g_m)^T \in R^m$, and m is the number of inequality constraints.

Robust Optimization Formulation

In this section, the robust optimization formulation for nonlinear optimization problems is developed. For simplicity, the model (2) with only inequality constraints is considered first and then the results are extended to the general case with both equality and inequality constraints as shown in (1). The most important issue in robust optimization is to define an uncertainty set for the uncertain parameters. There are various types of uncertainty set which leads to different robust counterpart formulations (Li et al., 2011). The widely used uncertainty set is defined by l_p-norm. This type of uncertainty set can be easily applied for unbounded uncertainty distribution. For bounded uncertainty, it is too conservative to construct an uncertainty set exceeding the bounded uncertain region. It is more meaningful to define an uncertainty set which is a subset of the bounded uncertainty region. While the uncertainty region is determined only by the bounds (i.e., interval) of each parameter, the corresponding robust optimization formulations for linear optimization problem were derived in Li et al. (2011) for independent uncertainty and in Yuan et al. (2016) for correlated uncertainty. In this work, a more general type of uncertainty set is considered, which is defined as the intersection of two norm-induced uncertainty sets:

$$S=\left\{ s \middle| \left\|M_1(s-s_1)\right\|_{p_1} \leq \Delta_1, \left\|M_2(s-s_2)\right\|_{p_2} \leq \Delta_2 \right\} \tag{3}$$

where M_1 and M_2 are invertible matrices representing information such as perturbation and correlation of the uncertain parameters, s_1 and s_2 are the center points of the two sets, p_1 and p_2 are norm parameters used in the two sets, and Δ_1 and Δ_2 are the set sizes.

Inequality-Only Case

The main idea of robust optimization is to enforce that constraints are satisfied for all the realizations of the uncertainty within the pre-defined uncertainty set S, which can be shown as:

$$G(u,s)\leq 0, \forall s \in S \tag{4}$$

which is equivalent to

$$\max_{s\in S} g_i(u,s) \leq 0, i=1,...,m \tag{5}$$

Before applying the robust optimization formulation, the nonlinear function g_i is linearized. Taking the first-order Taylor approximation in a small region around point s_*, we can obtain

$$\begin{aligned} & g_i(u,s) \approx g_i(u,s_*) + (s-s_*)^T \nabla_s g_i(u,s_*) \\ & = g_i(u,s_*) - {s_*}^T \nabla_s g_i(u,s_*) + s^T \nabla_s g_i(u,s_*) \leq 0 \end{aligned} \tag{6}$$

where $\nabla_s g_i$ denotes the gradient of g_i with respect to s. The robust constraint (5) can be approximated as

$$\begin{aligned} & \max_{s\in S} g_i(u,s) \\ & \approx g_i(u,s_*) - {s_*}^T \nabla_s g_i(u,s_*) + \max_{s\in S} s^T \nabla_s g_i(u,s_*) \leq 0 \end{aligned} \tag{7}$$

Apply the uncertainty set in Eq. (3), the inner maximization problem in (7) can be formulated as

$$\max_s \left\{ \begin{array}{l} s^T \nabla_s g_i(u,s_*): \\ \left\|M_1(s-s_1)\right\|_{p_1} \leq \Delta_1, \left\|M_2(s-s_2)\right\|_{p_2} \leq \Delta_2 \end{array} \right\}$$

(8)

The inner maximization problem is a conic programming problem, and by applying conic duality, the problem can be formulated as

$$\min_{w_1,w_2} \left\{ \begin{array}{l} -{s_1}^T M_1^T w_1 + \Delta_1 \|w_1\|_{q_1} \\ -{s_2}^T M_2^T w_2 + \Delta_2 \|w_2\|_{q_2} : \\ M_1^T w_1 + M_2^T w_2 = -\nabla_s g_i(u,s_*) \end{array} \right\} \tag{9}$$

where w_1 and w_2 are dual variables, and q_1 and q_2 are dual norm parameters, which satisfy $1/p_1 + 1/q_1 = 1$, $1/p_2 + 1/q_2 = 1$.

After some substitutions and variable replacements, the robust counterpart of the original inequality constraint is shown as follows

$$\begin{array}{l} g_i(u,s_*) - {s_*}^T \nabla_s g_i(u,s_*) \\ + {s_1}^T \nabla_s g_i(u,s_*) + ({s_2}^T - {s_1}^T) z \\ + \Delta_1 \left\| M_1^{-T}(z - \nabla_s g_i(u,s_1)) \right\|_{q_1} + \Delta_2 \left\| M_2^{-T} z \right\|_{q_2} \leq 0 \end{array} \tag{10}$$

where z is an auxiliary variable.

General Case

In the general case, state variables and equality constraints are involved in the nonlinear optimization. The state variables can be determined as a function of design variables and the uncertain parameter under the Implicit Function Theorem. First, we define $F_y(y,u,s)$ as the partial Jacobian of $F(y,u,s)$ with respect to y, i.e.,

$$[F_y(y,u,s)]_{ij} = \frac{\partial F_i(y,u,s)}{\partial y_j}$$

F_s, G_y, G_s, y_s are defined similarly. The state variable y can be implicitly defined as a function $y(u,s)$ through the state equation $F(y,u,s) = 0$. Apply the implicit function $y(u,s)$ in the inequality constraint, we have

$$G(u,s) = G(y(u,s),u,s) \tag{11}$$

Differentiating both sides of the equation $F(y(u,s),u,s) = 0$ with respect to s leads to the matrix equation

$$F_y(y,u,s)y_s + F_s(y,u,s) = 0 \tag{12}$$

Notice that $y(u,s)$ is an implicit function. It is not necessary to get an explicit expression of y_s, instead, it is treated as variables in the formulation. Differentiating $G(u,s)$ with respect to s, we have

$$G_s(u,s) = G_y(y,u,s)y_s + G_s(y,u,s) \tag{13}$$

For each individual inequality constraint i, the derivative is obtained as

$$\nabla_s g_i(u,s_*)^T = e_i^T G_s(u,s) = e_i^T [G_y(y,u,s)y_s + G_s(y,u,s)] \tag{14}$$

where e_i is the ith column of the identity matrix, and G_y, G_s takes value at s_*. Substitute Eq.(14) into the formulation shown in Eq.(10) and combining with the constraint shown in Eq.(12), the robust optimization for the general case is obtained

$$\begin{array}{ll} \min\limits_{y,u\in U} & \phi(y,u) \\ s.t. & F(y,u,s_*) = 0 \\ & F_y y_s + F_s = 0 \\ & g_i(y,u,s_*) + ({s_1}^T - {s_*}^T)(G_y y_s + G_s)^T e_i + ({s_2}^T - {s_1}^T) z \\ & + \Delta_1 \left\| M_1^{-T}(z - (G_y y_s + G_s)^T e_i) \right\|_{q_1} + \Delta_2 \left\| M_2^{-T} z \right\|_{q_2} \leq 0 \\ & i = 1, ..., m \end{array} \tag{15}$$

Iterative Algorithm

Since the first-order Taylor linearization around a single point is effective only in a small range, the robust optimization formulation derived in the third section works well only under small uncertainty region. If the perturbation is large, the linearization will be applied around multiple realizations (with index k) of the uncertain parameter. The robust optimization formulation for the general case is summarized in Eq.(16)

$$\begin{array}{ll} \min\limits_{y_m,u\in U} & \phi(y_m,u) \\ s.t. & F(y^k,u,s_*^k) = 0, \forall k \\ & F_y^k y_s^k + F_s^k = 0, \forall k \\ & g_i(y^k,u,s_*^k) + ((s_1^k)^T - (s_*^k)^T)(G_y^k y_s^k + G_s^k)^T e_i \\ & + ((s_2^k)^T - (s_1^k)^T) z^k + \Delta_2^k \left\| (M_2)^{-T} z^k \right\|_{q_2} \\ & + \Delta_1^k \left\| (M_1^k)^{-T}(z^k - (G_y^k y_s^k + G_s^k)^T e_i) \right\|_{q_1} \leq 0, \\ & i = 1, ..., m, \forall k \\ & y^k \leq y_m, \forall k \end{array} \tag{16}$$

All the constraints and corresponding variables in Eq.(15) are extended with respect to the multiple points around which the "piecewise" linearization is taken. The design variables u remains the same for all the points.

As shown in Eq.(16), if the state variable exists in the objective function, it is replaced by the maximum y_m of it among all the multiple points.

Another issue is how to select the points around which the "piecewise" linearization is taken. In this paper, the points are randomly selected within the uncertainty region, then feasibility is tested and an iterative algorithm is used to solve the problem. The algorithm is shown in Figure 1.

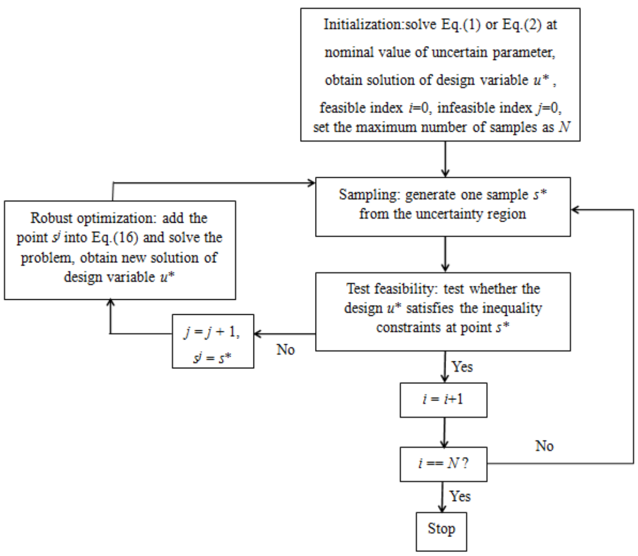

Figure 1. The iterative algorithm for solving the problem

Optimal Design of a Reactor-Separator System

In this section, a reactor design problem is studied to test the effectiveness of the proposed methodology. The optimal process design problem contains both inequality and equality constraints associated with uncertain parameters. The robust optimization formulations in the iterative algorithm are solved in GAMS. In the feasibility test step, the values of state variables are obtained by solving the state equations with fixed design variables and uncertain parameter values in MATLAB.

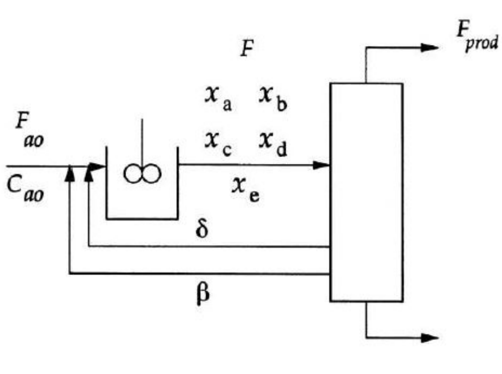

Figure 2. Reactor-separator process

A reactor design problem studied by Rooney and Biegler (2001) and Hale and Zhang (2007) is shown in Figure 2.

$$\begin{array}{ccccc} A & \xrightarrow{k_1} & B & \xrightarrow{k_2} & C \\ k_3 \downarrow & & k_4 \downarrow & & \\ D & & E & & \end{array}$$

The purpose of the system is to convert reactant A to product C via the above reaction system which consists of four first-order elementary reactions. The uncertain parameters are the reaction rates k_i, $i = 1, ..., 4$ with units of $time^{-1}$, i.e., $s = (k_1, k_2, k_3, k_4)^T$. The volume V of the reactor (m^3), the fraction δ of species A and B that is recycled back to the reactor, the fraction β of species D and E that are recycled back to the reactor are classified as design variables, i.e., $u = (V, \delta, \beta)^T$. The flow rate F out of the reactor ($mol/time$), the mole fraction of each species x_a, x_b, x_c, x_d, x_e at the reactor outlet is regarded as state variables, i.e., $y = (F, x_a, x_b, x_c, x_d, x_e)^T$. To minimize the total cost, the following optimization problem is formulated:

$$\begin{aligned} & \min 10V^2 + 5F \\ & s.t. \\ & F_{a0} - x_a F(1-\delta) - c_{a0} V(k_1 + k_3) x_a = 0 \\ & -x_b F(1-\delta) + c_{a0} V(k_1 x_a - (k_2 + k_4) x_b) = 0 \\ & -x_c F + c_{a0} V k_2 x_b = 0 \\ & -x_d F(1-\beta) + c_{a0} V k_3 x_a = 0 \\ & -x_e F(1-\beta) + c_{a0} V k_4 x_b = 0 \\ & x_a + x_b + x_c + x_d + x_e = 1 \\ & x_c F \geq 40 \\ & 0 \leq \delta \leq 1, 0 \leq \beta \leq 1 \end{aligned} \tag{17}$$

The known parameters are the inlet flow rate $F_{a0} = 100 mol/time$ and the concentration of species A at the inlet (the molar concentration throughout the entire system as well) $c_{a0} = 10 mol/m^3$. The detailed information about the uncertain parameters can be found in Rooney and Biegler (2001). Two types of uncertainty region which can be referred to as individual confidence region and joint confidence region are considered in this example. The uncertainty sets defined following Eq.(3) for individual confidence region (which is a box set) can be represented as Eq.(18):

$$S^j = \left\{ s \middle| \left\| s - s_*^j \right\|_\infty \leq \Delta, \left\| s - \hat{s} \right\|_\infty \leq t_{1-(\alpha/2),n-p}\sigma \right\}, \forall j \tag{18}$$

where σ is the standard derivation of the uncertain parameter, $t_{1-(\alpha/2),n-p}$ is the value of the Student-t distribution, α is the desired confidence level, p is the number of uncertain parameters, and n is the number of data points used in the estimation problem. The uncertainty set for joint confidence region is defined as

$$S^j = \left\{ \begin{array}{l} s \left| \left\| s - s_*^j \right\|_\infty \leq \Delta, \right. \\ \left\| \Sigma^{-1/2}(s - \hat{s}) \right\|_2 \leq (pF_{1-\alpha,n-p})^{1/2} \end{array} \right\}, \forall j \quad (19)$$

where Σ is the covariance matrix of the uncertain parameters, and $F_{1-\alpha,n-p}$ is the value of the F-distribution. Notice that the joint confidence region is an ellipsoid.

The solutions obtained by the "single-point" linearization are shown in Table 1 (Hale and Zhang, 2007).

Table 1. "Single-point" linearization (Hale and Zhang, 2007)

Set type	V (m^3)	δ	β	Cost
Box	20.71	0.992	0.000	6632
Ellip.	19.57	0.978	0.000	5983

In this example, we also test the results for different set sizes Δ (0.005, 0.01, 0.02, 0.05 for individual confidence region and 0.005, 0.01, 0.02 for joint confidence region), and for each set size, 100 Monte Carlo runs are taken. The average value (Ave), the maximum value (Max), and the minimum value (Min) of the objective value (Obj) and the number of points (Num) used for "piecewise" linearization among 100 Monte Carlo runs for individual confidence region and joint confidence region are listed in Table 2 and Table 3, respectively.

Table 2. Results for reactor-separator example (individual confidence region)

Size	Obj			Num		
Δ	Ave	Max	Min	Ave	Max	Min
0.005	6393.1	6645	6221	3.68	5	1
0.01	6388.3	6672	6171	2.64	4	1
0.02	6375.5	6681	6108	1.86	3	1
0.05	6403.1	6769	6133	1.8	3	1

Table 3. Results for reactor-separator example (joint confidence region)

Size	Obj			Num		
Δ	Ave	Max	Min	Ave	Max	Min
0.005	6195.1	6490	5865	2.04	3	1
0.01	6182.8	6674	5800	1.41	2	1
0.02	6290.2	6616	5922	1	1	1

By comparing the results in both Table 2 and Table 3, it can be seen that as the set size increases, the number of points needed for linearization decreases. However, for the objective values, the best results for the individual confidence region and joint confidence region are obtained at size 0.02 and size 0.01 by comparing the average value. In addition, the results show that the size Δ can be optimized to obtain better results.

Comparing the results obtained by the "piecewise" linearization and "single-point" linearization, it can be observed that for the individual confidence region case, although the maximum objective value in Table 2 is slightly larger than the objective value in Table 1, the average value is much smaller than the results in the literature.

The robustness of the solutions is tested using 100 samples. The simulation results are plotted in Figure 3 and Figure 4.

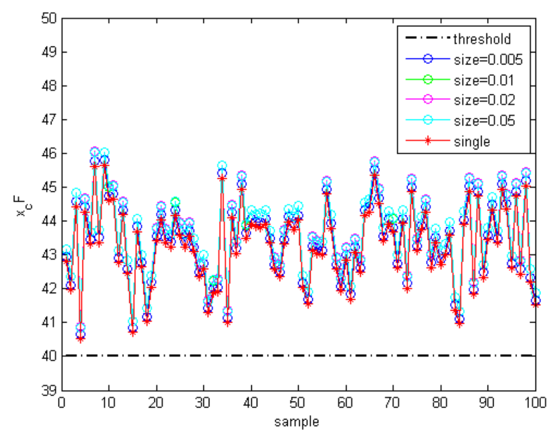

Figure 3. Results for individual confidence region

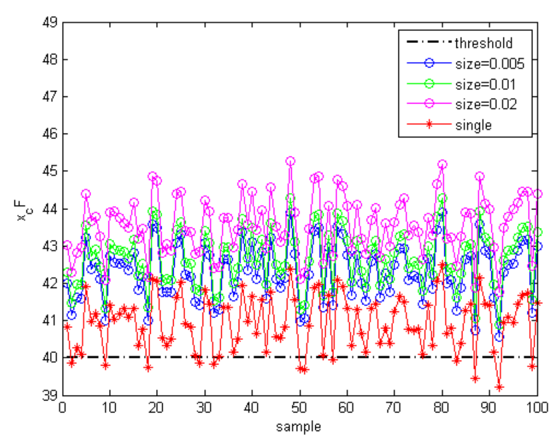

Figure 4. Results for joint confidence region

The number of samples violating the constraints for the "piecewise" linearization method are all zeros for both individual confidence region and joint confidence region cases. While for the "single-point" linearization method, the numbers of violation samples is 12 for joint confidence region and 0 for individual confidence region. Although in the joint confidence region case, the objective for the "single-point" linearization is better than the one for "piecewise" linearization, and the robustness is worse. For the constraints, if the corresponding curve is closer to the threshold the results is less conservative. In Figure 3, the lines for size 0.01, 0.02, and 0.05 coincide and they are slightly more conservative than the results for size 0.005. In Figure 4, as the size increases, the results become more conservative with respect to the constraints. This observation may also be useful for the selection of the set size.

Conclusion

In this paper, a novel nonlinear robust optimization framework was proposed to solve the nonlinear process design problems under uncertainty. The robust counterpart formulation is derived based on a general type of uncertainty set defined by the intersection of two uncertainty sets. In order to deal with uncertainty with larger perturbation, "piecewise" linearization is taken around multiple realizations of the uncertain parameter and an iterative algorithm is applied to solve the problem. The framework is applicable for the optimization problems with only inequality constraints as well as the problems with equality constraints associated with uncertain parameters. For problems where uncertain parameters exist in equality constraints as well, the traditional robust optimization method cannot be directly applied. However, the state variables can be determined while the design variables and the uncertain parameters are fixed. Based on the Implicit Function Theorem, the state variables can be replaced by a function of uncertain parameters and design variables. Then the robust optimization formulation can be applied on the inequality constraint after eliminating the state variables. An optimal process design example is studied to demonstrate the effectiveness of the proposed methodology. The results show that the proposed method has a higher level of robustness than the "single-point" linearization method. In addition, while the results have the similar robustness level, the proposed method leads to less conservative robust solution.

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References

Ben-Tal, A., El Ghaoui, L., and Lebret, H. (1998). Robust semidefinite programming. *Handbook on Semidefinite Programming*, 27.

Ben-Tal, A. and Nemirovski, A. (1999). Robust solutions of uncertain linear programs. *Operations research letters*, 25(1):1–13.

Ben-Tal, A., Nemirovski, A., and Roos, C. (2002). Robust solutions of uncertain quadratic and conic-quadratic problems. *SIAM Journal on Optimization*, 13(2):535–560.

Bertsimas, D. and Sim, M. (2004). The price of robustness. *Operations research*, 52(1):35–53.

Diehl, M., Bock, H. G., and Kostina, E. (2006). An approximation technique for robust nonlinear optimization. *Mathematical Programming*, 107(1-2):213–230.

El Ghaoui, L. and Lebret, H. (1997). Robust solutions to least-squares problems with uncertain data. *SIAM Journal on Matrix Analysis and Applications*, 18(4):1035–1064.

El Ghaoui, L., Oustry, F., and Lebret, H. (1998). Robust solutions to uncertain semidefinite programs. *SIAM Journal on Optimization*, 9(1):33–52.

Hale, E. T. and Zhang, Y. (2007). Case studies for a first-order robust nonlinear programming formulation. *Journal of optimization theory and applications*, 134(1):27–45.

Li, Z., Ding, R., and Floudas, C. A. (2011). A comparative theoretical and computational study on robust counterpart optimization: I. robust linear optimization and robust mixed integer linear optimization. *Industrial & engineering chemistry research*, 50(18):10567–10603.

Rooney, W. C. and Biegler, L. T. (2001). Design for model parameter uncertainty using nonlinear confidence regions. *AIChE Journal*, 47(8):1794–1804.

Yuan, Y., Li, Z., and Huang, B. (2016). Robust optimization under correlated uncertainty: Formulations and computational study. *Computers & Chemical Engineering*, 85:58–71.

Zhang, Y. (2007). General robust-optimization formulation for nonlinear programming. *Journal of optimization theory and applications*, 132(1):111–124.