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Comprehensive Sensitivity Analysis in NLP Models in PSE Applications Using Space-Filling DOE Strategy

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Sensitivity analysis is an integral step in the interpretation of the solutions of optimization models, particularly when there are uncertainties in the numerical values of model parameters. Conventional approaches to sensitivity analysis rely on the use of shadow prices in linear models and Lagrange multipliers in non-linear models. Modern commercial optimization software packages are able to automatically generate such sensitivity coefficients to allow rapid post-optimality analysis. However, in the case of non-linear models, Lagrange multipliers have two distinct limitations. First, they represent only changes in the optimal value of an objective function with respect to small changes in parameter values, and thus remain valid only near the immediate vicinity of the nominal design point. Secondly, each Lagrange multiplier gives only the effect of the change of one parameter, assuming that all other parameters remain at their nominal values. Hence, they provide no information about joint effects or interactions caused by simultaneous changes in parameter values. In this paper, we present a strategy based on design of experiments (DOE) to generate a sensitivity surface, which we define as the mapping of the optimal model solution against a range of values of the optimization model parameters. Space-filling designs are used as a basis to generate proxy regression models with quadratic and interaction terms, in order to capture curvature of the sensitivity surface. The resulting proxy model contains more information than is available in conventional sensitivity analysis. In particular, this approach shows curvature and interaction effects that are not reflected when Lagrange multipliers are used. We present case studies based on problems drawn from process systems engineering (PSE) literature to illustrate this comprehensive sensitivity analysis strategy.

1. Introduction

Optimization models have been used in chemical engineering design problems since the 1950s (Fenech and Acrivos, 1956). Mathematical programming techniques have become an essential tool in process systems engineering (PSE) in general (Stephanopoulos and Reklaitis, 2011), and process synthesis specifically (Cremaschi, 2014). Optimization methods are used nowadays in conjunction with process simulation software (e.g., Sun et al., 2014). Initial approaches dealt with deterministic models whose parameter values were assumed to reflect precisely known physical or economic quantities. However, it eventually became clear that uncertainties are inherently present when mathematical models are used to represent real systems; as a result, different approaches have been developed for dealing with uncertainties. For example, sensitivity analysis around the optimal results can be used (Seferlis and Hrymak, 1996). Such capabilities are usually available as a default feature in commercial optimization software. A wide array of optimization methodologies, such as stochastic programming, fuzzy programming, chance-constrained programming, etc. – have also been proposed for various PSE problems (Sahinidis, 2004).
Conventional sensitivity analysis features found in commercial optimization software focus on determining shadow prices (for linear programs or LPs) or Lagrange multipliers (for nonlinear programs or NLPs), both of which give the local sensitivity of the optimal solution to infinitesimal changes in values of the constant term in each constraint individually. Note that this definition results in two limitations. First, this form of

sensitivity analysis is only applicable for exploring the immediate vicinity of a nominal optimum, while, in practice, the degree of sensitivity will often change for finite deviations from this point. Second, each sensitivity coefficient gives the ratio of change in optimal value per unit change in a given parameter, assuming all other parameters remain fixed at their nominal values. Thus, joint effects, or interactions, are not reflected in such results.
In this paper, we propose a sampling-based sensitivity analysis procedure for process synthesis models in PSE applications using space filling experimental designs. Such techniques have been developed to allow design of experiment (DOE) philosophy to be applied to various forms of "computational experiments" (e.g., Ye, 1998). The rest of this paper is organized as follows. Section 2 discusses the methodology based on space-filling experimental designs. Next, Sections 3 and 4 illustrate the approach using two benchmark problems from PSE literature. The sensitivity analysis approach used here is compared with standard analysis via Lagrange multipliers. Concluding remarks and prospects for future work are then given in Section 5.

2. Methodology

The sampling-based sensitivity analysis approach proposed here is based on the Latin hyperube space filling design proposed by Ye (1998). As with other space filling designs, this approach makes use of experimental points dispersed through an *n*-dimensional factor space, as illustrated in Figure 1.

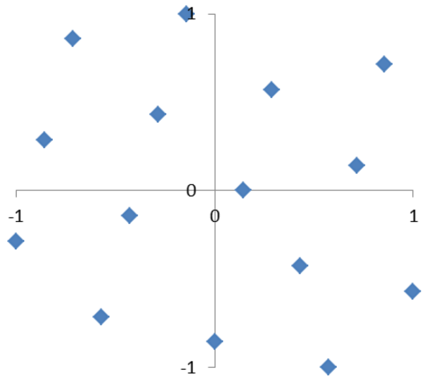

Figure 1: A two-factor Latin hypercube design with 15 runs

The general procedure is as follows:

- Consider an optimization model with objective function *f*(**x**) and decision variable vector **x,** whose optimal solution is *f*(**x***)
- Assume that the model contains *n* uncertain or imprecise parameters, given by vector **b**, whose elements are limited by lower bound vector $\mathbf{b}_L$ and upper bound vector $\mathbf{b}_U$
- The uncertain parameters thus define an *n*-dimensional factor space, such that a unique optimal solution can potentially be found for each point within the factor space
- A Latin hypercube space filling design is used to sample the factor space with enough points to ensure sufficient degrees of freedom for subsequent statistical analysis
- The optimization model is solved in turn for each point in the design
- A proxy polynomial regression model is then derived empirically from the solutions found in the previous step; this model gives a statistically significant estimate of *f*(**x***) as a function of **b**, thus allowing the optimal solution of the original model to be predicted for any value of **b** without having to re-solve it further

The methodology is illustrated in the succeeding sections using two benchmark NLP problems from PSE literature. The optimization models are solved using LINGO 13.0 developed by Lindo Systems. This software is equipped with a Global Solver utilizing a branch-and-bound algorithm (Gau and Schrage, 2003) for solving non-linear models. The generation of the space-filling experimental designs, and subsequent data analysis to generate the proxy regression models, are accomplished using JMP Pro v.11 developed by SAS.

3. Case Study 1

This simplified process plant flowsheet optimization example is based on the NLP problem by Stephanopoulos and Westerberg (1975), as described in the compilation of benchmark problems by Ryoo and Sahinidis (1995). The NLP formulation is:

minimize $x_1^{0.6} + x_2^{0.6} - 6\,x_1 - 4\,x_3 + 3\,x_4$ (1a)

subject to:

$-3\,x_1 + x_2 - 3\,x_3 = 0$ (1b)

$x_1 + 2\,x_3 \leq F_1$ (1c)

$x_2 + 2\,x_4 \leq F_2$ (1d)

$0 \leq x_1 \leq 3$ (1e)

$0 \leq x_2 \leq 4$ (1f)

$0 \leq x_3 \leq 2$ (1g)

$0 \leq x_4 \leq 1$ (1h)

where the numerical values of two of the model parameters are given by the intervals $F_1 \in [3.8, 4.2]$ and $F_2 \in [3.8, 4.2]$. The objective function corresponds to minimization of total cost (Eq 1a). In the original model, $F_1 = F_2 = 4$ and the optimal objective function value is -4.514. A Latin hypercube design with eight points was generated and the model solved for each design point. Then, the an empirical 2nd-order polynomial regression model with two-factor interaction terms was derived from this data, using F_1 and F_2 as factors, and the optimal objective function value as the response. Table 1 shows the term-by-term statistical analysis of this proxy model. Note that p-values of 0.05 or less signify statistically significant effects, while the parameter signs indicate the direction of the effect. Figure 1 shows the behaviour of the optimal objective function value as a function of F_1 and F_2. Note the pronounced response surface curvature and inflection, as a consequence of the statistically significant quadratic and interaction terms. Such effects cannot be clearly indicated by conventional sensitivity analysis; for instance, in this case, when $F_1 = F_2 = 4$, the Lagrange multipliers for Eq(1c) and (1d) are both zero.

Table 1: Effect of model parameters F_1 and F_2 on optimal objective function value

Term	Estimate	p-value	Remark
F_1	0*	> 0.05	Not statistically significant
F_2	–0.147	< 0.0001	Statistically significant negative effect
F_1^2	–0.004	0.0069	Statistically significant negative effect
F_2^2	+0.156	< 0.0001	Statistically significant positive effect
F_1F_2	–0.040	< 0.0001	Statistically significant negative effect

*Statistically insignificant terms effectively have zero value

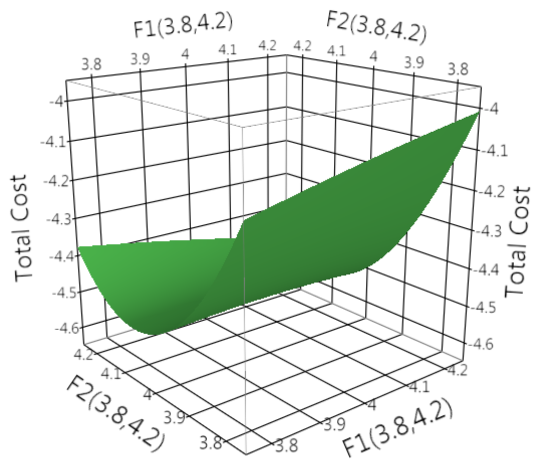

Figure 2: Response surface of optimal Total Cost as a function F_1 and F_2

4. Case Study 2

This Heat Exchanger Network example is based on the NLP model of Liebman et al. (1986), as modified by Ryoo and Sahinidis (1995). The NLP formulation is:

minimize $x_1 + x_2 + x_3$ (2a)

subject to:

$100,000\ (x_4 - 100) = U_1\, x_1\, (300 - x_4)$ (2b)

$100,000\ (x_5 - x_4) = U_2\, x_2\, (400 - x_5)$ (2c)

$100,000\ (500 - x_5) = U_3\, x_2\, (600 - 500)$ (2d)

$0 \le x_1 \le 15,834$ (2e)

$0 \le x_2 \le 36,250$ (2f)

$0 \le x_3 \le 10,000$ (2g)

$0 \le x_4 \le 300$ (2h)

$0 \le x_5 \le 400$ (2i)

where the numerical values of three of the model parameters are given by the intervals $U_1 \in [114, 126]$, $U_2 \in [76, 84]$ and $U_{23} \in [38, 42]$. It is assumed here that uncertainties in the problem arise from imprecise estimation of the heat transfer coefficients for the network. The objective function is to minimize total heat transfer are (Eq. 2a). As reported by Ryoo and Sahinidis (1995), the optimal solution is 7,049.25 at the central point of the factor space, with $U_1 = 120$, $U_2 = 80$ and $U_3 = 40$.

Using a Latin hypercube design with 15 points, the proxy regression model with linear, quadratic and two-facto interaction term was derived to predict optimum heat transfer area as a function of U_1, U_2 and U_3. Statistical analysis of the regression model is given in Table 2. Note that all linear effects are statistically significant with negative values, which results from the inverse influence of heat transfer coefficient on heat transfer area. For higher-order effects, only the quadratic and interaction terms corresponding to U_2 and U_3 are statistically significant. Response surfaces of optimal total area plotted against U_1 and U_2, U_1 and U_3, and U_2 and U_3 are given in Figures 3, 4 and 5. It can be clearly seen in Figure 5 that, unlike in the previous case study, the curvature of the response surface has a small magnitude despite being statistically significant. For purposes of sensitivity analysis, the quadratic and interaction terms may thus have negligible influence.

Table 2: Effect of model parameters U_1, U_2 and U_3 on optimal objective function value

Term	Estimate	p-value	Remark
U_1	−28.8	< 0.0001	Statistically significant negative effect
U_2	−67.8	< 0.0001	Statistically significant negative effect
U_3	−255.7	< 0.0001	Statistically significant negative effect
U_2^2	+1.4	0.0184	Statistically significant positive effect
U_3^2	+10.4	< 0.0001	Statistically significant positive effect
U_2U_3	+2.4	0.0008	Statistically significant positive effect

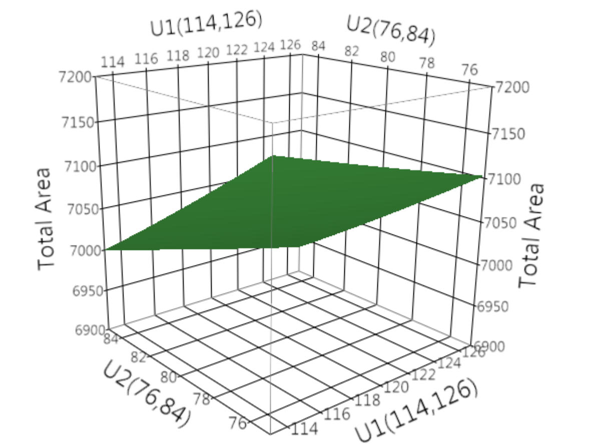

Figure 3: Response surface of optimal Total Area plotted against U_1 and U_2

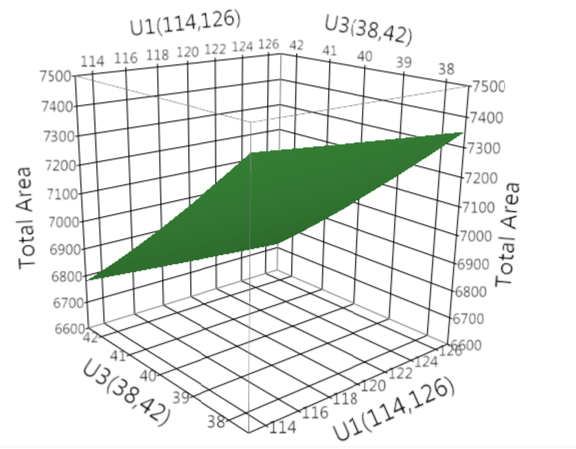

Figure 4: Response surface of optimal Total Area plotted against U_1 and U_3

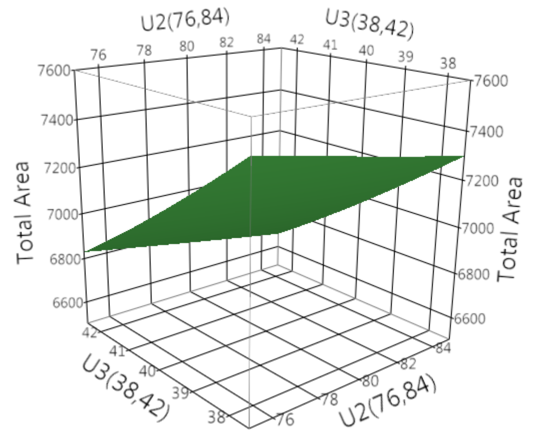

Figure 5: Response surface of optimal Total Area plotted against U_2 and U_3

5. Conclusions

This paper has proposed a comprehensive sensitivity analysis procedure for NLP models in PSE applications using space-filling experimental designs. The approach is based on the empirical generation of proxy models that predict the optimal objective function value as a function of the numerical values of the base model parameters. Unlike conventional sensitivity analysis based on Lagrange multipliers, this approach allows non-linear effects and interactions to be detected over an arbitrary range of parameter values. As proof of concept, two benchmark PSE case studies have been solved to illustrate this approach, based on Latin hypercube designs. Future work will focus on further testing of this methodology on a broader range of PSE problems. Aspects such as computational efficiency for different types of space-filling experimental designs applied to large-scale models can also be assessed.

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