

Worst-Case Responses Estimate Impact on Pareto Front

Nuno COSTA* and João LOURENÇO

Instituto Politécnico de Setúbal – Escola Superior de Tecnologia de Setúbal

Centro de Desenvolvimento de Produto e Transferência de Tecnologia, 2910-761 Setúbal, Portugal

*Corresponding author

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Abstract. For a reasoned decision-making in multiresponse problems, it is important to investigate how consistent the Pareto Frontier is to responses estimation uncertainty. To investigate the impact of this uncertainty source on the Pareto frontier, solutions achieved from the worst and mean responses estimate were generated and compared. Results are displayed graphically and a metric is used to select an optimal solution.

Introduction

Processes and products have multiple characteristics or properties (responses) that must be optimized simultaneously. In contrast to single response optimization problems, where the optimal solution is defined easily, for multiple responses optimization problems, a solution is more of a concept than a definition [1]. In practice, a collection of optimal or nondominated solutions from where the decision-maker shall select one based on its preference or solution's impacts on product and process performance is generated from models built on mean estimated responses. However, it is known that models fitted to responses are, by nature, inaccurate due to process natural variability and estimation uncertainty of model's coefficients. This has implications on the generated (optimal or Pareto) solutions and on their characteristics, namely on the solutions reproducibility, which has also been not addressed in the literature. Thus, in contrast to the current practice, solutions reproducibility is assessed here through a novel metric, and Pareto frontiers generated from the mean and worst responses estimates are evaluated.

Solutions Generation and Dominance Relation

To conduct statistically designed experiments for modelling the responses surface and use a function that combines the models of multiple responses for finding a solution that either maximizes or minimizes the aggregated function is a frequent practice in the RSM framework that has been illustrated by several authors, namely in [2-5], as examples. However, for multiresponse optimization (MRO) problems there is not a unique solution that is best (global minimum or maximum) with respect to all responses. In practice, the utopia point (the variables setting that would yield all responses at

thus, a compromise solution must be identified, and a desired condition for any candidate solution is to be non-dominated.

Pareto optimality is a predominant concept in defining a non-dominated solution. For a minimization problem like that formulated in (1),

$$\text{Minimize } F(\mathbf{x}) = [f_1(\mathbf{x}), \dots, f_p(\mathbf{x})] \quad (1)$$

subject to

$$G(\mathbf{x}) = [g_1(\mathbf{x}), \dots, g_q(\mathbf{x})] < 0$$

$$H(\mathbf{x}) = [h_1(\mathbf{x}), \dots, h_w(\mathbf{x})] = 0$$

$$x_m^l \leq x_m \leq x_m^u$$

where the objective function, inequality and equality constrained functions are denoted by $F(x)$, $G(x)$ and $H(x)$, respectively; the x_m is the vector of input variables or decision vector, with lower and upper bounds denoted, respectively, by x_m^l and x_m^u , a solution x_1 is said to dominate another solution x_2 , if both the following conditions are true:

$$a) \quad f_i(x_1) \leq f_i(x_2) \quad \forall i \in 1, \dots, p;$$

$$b) \quad \exists j \in 1, \dots, p : f_j(x_1) < f_j(x_2).$$

Non-dominated solutions, namely the called Pareto frontiers, are usually generated from least squares point estimates of the responses at a given set of input variables (hereafter referred to as the ‘‘mean model’’) without considering the uncertainty in the parameter estimates. Since the responses are likely to have different natural variability in the region of operation, the precision with which the parameters are estimated differs, making it difficult to anticipate effects on the Pareto frontier solutions [6]. One cannot also ignore that sampled data are another source of uncertainty in estimating the response surfaces. Another set of collected data would yield different response surfaces and, consequently, another Pareto frontier would be generated. Such as Chapman et al. [6] noted, naively treating the estimated response surfaces as fixed can lead to overconfidence in the conclusions and potentially sub-optimal input factor level choices that do not yield the expected practical results.

Here, the Pareto frontier is generated from

i) response estimate at input variable settings (x_i) are defined as

$$\hat{f}_i(x_m) = x_m^T \hat{\beta}, \quad (2)$$

where $\hat{\beta}$ represents the estimated model parameters (coefficients of the response mean model);

ii) response estimate at input variable settings are defined as

$$\hat{f}_i(x_m) = x_m^T \hat{\beta} \pm t_{\alpha/2, n-z} \sqrt{MSE(1 + x_m^T (X'X)^{-1} x_m)}, \quad (3)$$

where the mean square error $MSE = SS_E/(n-z)$, SS_E is the error sum of squares, n is the number of experimental runs in the model matrix X , z is the number of terms in the response’s model, and α is the significance level [7]. Note that, in this manuscript, it is always considered the worst-case estimates for responses. This means that when a response must be maximized (is a Larger-The-Better response type - the estimated response value is expected to be equal or larger than an upper bound) a minus sign is used in (3) whereas a plus sign is used for responses which must be minimized (is a Smaller-The-Better response type - the value of the estimated response is expected to be equal or smaller than a lower bound). For a Nominal-The-Best (NTB) response type (the estimated response value is expected to be equal to a target value) a plus or minus signal can be used in (3), depending on which one makes the response estimate value far from target.

When the Pareto frontier generated from the estimated mean responses (as in (2)) significantly differ from that generated from the estimated worst responses (as in (3)), the decision-maker can use the quality of predictions (QoP) metric proposed by Costa and Lourenço [4] to identify a solution with high reproducibility (lower QoP value). When Ordinary Least Squares regression technique is used to fit models to responses,

$$QoP = trace[\varphi \Sigma_{\hat{y}}(x^*)], \quad (4)$$

where φ is a matrix whose elements are $\varphi_{ii} = 1/(U_i - L_i)^2$ and $\varphi_{ij} = 1/(U_i - L_i)(U_j - L_j)$ for $i \neq j$, with $i, j = 1, \dots, n$, and $\Sigma_{\hat{y}}(x^*)$ represents the variance-covariance matrix of the n estimated responses at optimal location x^* . If all the models fitted to responses have the same regressors, one can write

$$\Sigma_{\hat{y}}(x^*) = x^{*T} (X'X)^{-1} x^* \hat{\Sigma}, \quad (5)$$

where X is the model matrix, $\hat{\Sigma} = \hat{e}_i^T \hat{e}_j^T / N$, \hat{e} represents the estimated residuals (difference between the observed response value and the corresponding estimated value) and N is the number of experimental observations. If the Seemingly Unrelated Regression technique is used, the reader is referred to [8] where a variant of the QoP metric is defined and illustrated.

The Pareto frontier (optimal solutions) are generated with a compromise programming-based criterion introduced in [9], varying the shape factor $1 \leq \omega_i \leq 12$ with increments of one unit, and a Sequential Quadratic Programming algorithm are used.

Example

This case study aimed at determining the settings for reaction time (x_1), reaction temperature (x_2), and amount of catalyst (x_3) for maximizing the conversion (y_1) of a polymer and achieving a target value for the thermal activity (y_2). A central composite design with four center points was run and the range values for y_1 and y_2 are [80, 100] and [55, 60], respectively [3]. The target value for y_1 was set equal to 100 and for y_2 was set equal to 57.5. The constraints for the input variables are $-1.682 \leq x_m \leq 1.682$ with $m = 1, 2, 3$ and the mean models fitted to responses, denoted by $\hat{\mu}_1$ and $\hat{\mu}_2$, according to [3], are as follows:

$$\hat{\mu}_1 = 81.0943 + 1.0290x_1 + 4.0426x_2 + 6.2060x_3 - 1.8377x_1^2 + 2.9455x_2^2 - 5.2036x_3^2 + 2.1250x_1x_2 + 11.3750x_1x_3 - 3.8750x_2x_3 \quad (R^2 = 0.9199; R_{Adj}^2 = 0.8478)$$

$$\hat{\mu}_2 = 59.8505 + 3.5855x_1 + 0.2547x_2 + 2.2312x_3 + 0.8360x_1^2 + 0.0742x_2^2 + 0.0565x_3^2 - 0.3875x_1x_2 - 0.0375x_1x_3 + 0.3125x_2x_3 \quad (R^2 = 0.8918; R_{Adj}^2 = 0.7944)$$

Figure 1 displays the Pareto frontier for both the mean and worst responses estimate, represented with crosses and circles, respectively. In this case, one can see a significant difference between the Pareto frontiers, though the data trend is similar, that is, the further away from the target τ_2 value is, the higher τ_1 value will be. Pareto frontier built on the mean estimated responses is widely used, but there is no guarantee that all these solutions are either equally “good” or better than those achieved from worst responses estimate. Further information is useful to validate it, namely the optimal solutions assessment in terms of solutions’ quality of predictions (see Figure 2), where it is apparent that some solutions reproducibility is undesirably lower (QoP is higher) as well as to investigate if optimal variable settings are significantly different for both Pareto frontiers. In this situation, significant differences are apparent (see Figure 3).

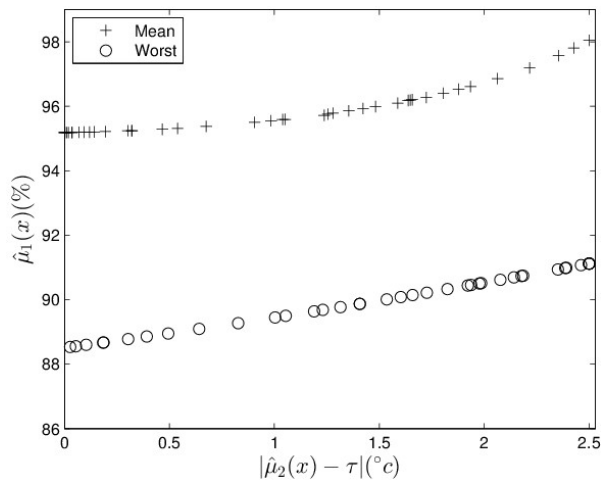


Figure 1. Pareto frontiers

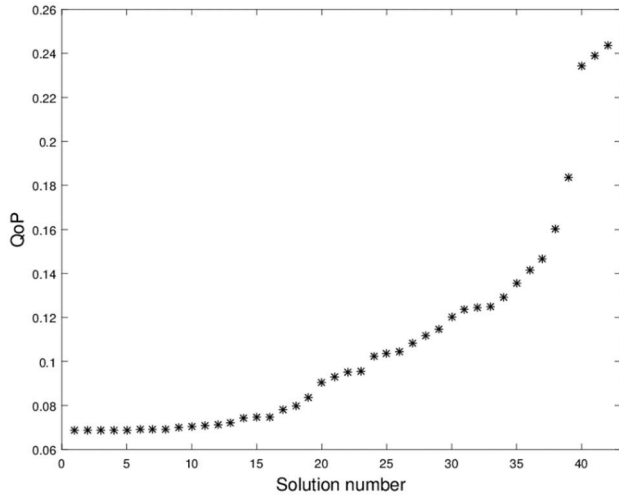


Figure 2. Quality of prediction

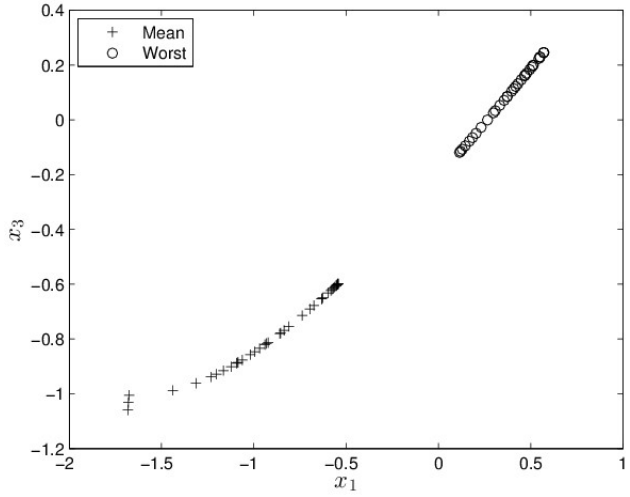


Figure 3. Optimal variable settings ($x_2 = 1.682$)

Results Discussion

To use the mean response models for generating the Pareto frontier and making decisions about the preferred solution in multiresponse problems is a procedure that ignores the uncertainty associated to the responses surface. If this uncertainty is not neglectable, there is no guarantee that future observed responses will be equal to the estimated responses when the process is run at a chosen design location. Such as Chapman et al. [6, 10] shown, natural variability in the process and subsequent uncertainty in the experimental values result in less accurate response models and different Pareto frontiers. In practical terms, this means that process or product performance will be not as good as it could be possible.

The example considered here shows that Pareto frontiers generated from mean and worst responses estimate are not similar (change is relevant). However, one can anticipate that Pareto frontiers did not change substantially when R^2 and Adjusted R^2 values are similar and large ($>95\%$). To gain a further understanding of how uncertainty can impact on the robustness of results, a simulation study to evaluate the Pareto frontiers change due to variability in the estimated response surfaces can be helpful. In fact, simulation-based studies can account for both the parameter estimates and the response model uncertainty, which helps to examine the variability impact on the Pareto frontier solutions and facilitates a more informed solution selection by the decision-maker. However, so far, this was rarely done because it takes too much time to compute and it is not sure that significantly better solutions will be found. Nevertheless, with the computing speed increasing, it may become a usual practice. For guidelines on it the reader is referred to [10].

To evaluate the Pareto frontier consistency for different levels of uncertainty in the data as part of the optimization process is important for realistic decision-making in multiresponse problems. A larger variety of scenarios or alternative optimal solutions will provide a further understanding of the problem as well as the impact of subjective choices in the optimization process, helping the decision-maker to take informed decisions more confidently.

We anticipate that there will be many situations where the Pareto frontiers built on the mean and worst estimates will differ significantly. In such situations, the decision-maker should carefully consider whether primary interest lies in focusing on average or worst-case performance, because the solutions reproducibility can't be ignored. To use the QoP metric is an appropriate approach to identify a solution with the highest reproducibility, which can be especially useful for problems with more than two responses.

Conclusion

This work goes beyond the current practice of displaying a Pareto frontier for a bi-objective problem by representing graphically the Pareto frontiers generated from both the mean and worst responses

estimate. This provides to the decision-maker a broader set of competing choices from where a unique solution should be selected and indications how changes in the responses variability are propagated to the Pareto frontier. The case study provides evidence that a larger uncertainty in the estimates of model's coefficients impact on Pareto frontier solutions, and hence less confidence the decision-maker may have in the reproducibility of selected solution. Nevertheless, more case studies are necessary to investigate how often this result can occur in real-life problems, though it is expected that higher natural variability and higher model's coefficients uncertainty more significant differences between the Pareto frontiers will occur.

Practitioners and decision-makers need to be aware that the mean model approximation is not a panacea and the uncertainty associated to some optimal solutions can be excessively high. Additional research is also welcoming to introduce tools or graphs for assessing the solutions reproducibility and guide the decision-maker in selecting confidently a solution among those of the Pareto frontier, namely for problems with a higher number of responses of distinct types. Nevertheless, the QoP metric presented can be useful.

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