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Assessing the resilience of optimal solutions in multiobjective problems

Nuno Costa [a,b,*], João Lourenço [a]

[a] Instituto Politécnico de Setúbal, ESTSetúbal; Campus do IPS, Estefanilha, 2910-761, Setúbal, Portugal
[b] UNIDEMI, NOVA School of Science and Technology, Universidade NOVA de Lisboa, 2829-516, Caparica, Portugal

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ABSTRACT

Processes and products are multidimensional so researchers and practitioners have to solve problems with multiple objectives frequently. These problems have, in general, responses in conflict so they do not have a unique solution. Different approaches have been proposed in the literature to solve these problems, but many of them, including the popular desirability function approach, are not employed with the focus on the generation of Pareto frontiers. In addition, it is important to stress that some Pareto solutions may not yield the expected outcome(s) when implemented in practice. Thus, to avoid wasting resources and time in implementing a theoretical solution which does not produce the expected outcome(s), in this paper is proposed a novel metric to assess the resilience of Pareto solutions. This way, the decision-maker may identify a solution less sensitive to changes in the variables setting when their values are implemented in production process (equipments) or during its operation. Metric usefulness is illustrated using a case study, and results analysis is complemented with plots that facilitate the decision-making process.

1. Introduction

Optimization in chemistry by manipulation of one variable at a time is no longer a predominant practice. Instead of it, multivariate statistic approaches have been often applied and Response Surface Methodology (RSM) is among the most popular ones, if not the most often used. In fact, this methodology and its advantages are thoroughly exposed in books as well as in scientific papers so there is no reason to ignore or misapply the RSM. Guidelines on the planning, conducting, and analysis of statistical designed experiments are reported, as example, in Refs. [1–3].

A usual problem faced by researchers and practitioners in all branches of chemistry is the simultaneous optimization of multiple objectives [4–9]. Aggregating the multiple objectives (responses) into a single optimization index is a current practice, and desirability function indexes are often used for this purpose. An extensive review on desirability functions is presented in Refs. [10,11], and a collection of works in chemistry where the most popular desirability function, the called Derringer & Suich desirability function is employed, is presented in Refs. [12,13]. Criticisms to these type of optimization functions are also reported in the literature, including the subjective information (weights and/or shape factors) required from the analyst or decision-maker and the non-optimality of generated solutions [14,15].

To validate the solution generated from the Derringer & Suich desirability function [16], which is predominant in the optimization of multiresponse problems [12,13], in chemistry and in many other science fields, most researchers and practitioners run one or more confirmatory experiments. However, this is done with no guaranty of the optimality or any technical evaluation of the selected solution in terms of its reproducibility. This may result in wasting resources and time if the selected solution does not yield the expected outcome (process or product improvement or conformance with the specifications) when it is implemented in production process (equipments), or during its operation. To avoid it, or at least to minimize the gap between theoretical and practical results, in this paper a new and easy-to-implement tool to assess the resilience of nondominated (Pareto) solutions, i.e., the sensitivity of Pareto solutions to changes in the input variables setting, including to truncation and rounding, is proposed.

The remaining of the paper is structured as follows: next section includes the framework to introduce the proposed metric to select Pareto solutions. Section 3 includes one case study to illustrate the usefulness of the proposed metric, and discuss the results. Conclusions are presented in Section 4.

* Corresponding author. Instituto Politécnico de Setúbal, ESTSetúbal; Campus do IPS, Estefanilha, 2910-761, Setúbal, Portugal.
E-mail addresses: nuno.costa@estsetubal.ips.pt (N. Costa), joao.lourenco@estsetubal.ips.pt (J. Lourenço).

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2. Materials and methods

When the objective is to optimize several responses, it is expected to have conflicting responses. For this purpose, a widely accepted and employed approach is the simultaneous optimization of multiple responses. A set of solutions, as complete as possible in terms of cardinality, uniformity, and coverage [17], where any improvement in one response cannot occur without degrading the value of, at least, another response, are of particular preference for those who want to solve multiresponse problems. These are called nondominated (Pareto optimal or simply Pareto) solutions. However, many of the nondominated solutions may lead to process operation conditions or process and product outputs that are less favourable in technical and/or economical terms [18,19].

The variety and quantity of optimization methods or criteria put forward in the RSM literature for solving multiresponse problems are large, however, the ability of those methods or criteria to depict Pareto frontiers has been rarely evaluated. Exceptions are [14,17,19–23]. Regarding the quality, or evaluation, of Pareto frontiers, the reader is referred to Refs. [24,25].

To represent the Pareto frontier in a plot may provide useful information to aid the decision-maker in interpreting the results and justifying his/her choice for a particular Pareto solution. Examples of graphical approaches includes the parallel coordinates plot [26], cluster mapping plot [27], Level Diagrams [28], synthesized efficiency plot [29], Desirability-Weight-Input-Volume (DWIV) plot [30] and mixture (ternary) plot [15]. To improve the n-dimensional Pareto fronts graphical analysis, the called asymmetric distance was proposed in Ref. [31]. Other solution selection strategy (procedure) based on one or more metrics has been an alternative. Examples of those metrics include:

i) the desirability synthesized efficiency [32];
ii) the Bias (the sum of the differences of normalized responses value to their target), the Quality of Predictions (response's variance due to models coefficients uncertainty), and Robustness (response's variance due to noise factors) [33,34];
iii) the prediction standard error metric, as alternative to Quality of Prediction metric [35];
iv) implementation error and its interaction with responses model coefficients uncertainty in addition to bias, quality of predictions, and robustness [36];
v) the Pareto Uncertainty Index [37];
vi) the sum of ranking differences [38];
vii) the Technique for Order Preference by Similarity to the Ideal Solution- TOPSIS [39];
viii) the Analytical Hierarchy Process- AHP [40].

Other proposed solution selection strategy are the following:

i) to consider in the objective function the correlation among noise factors and intermediate response variables [41];
ii) take into account the experimental or estimation errors (related to unknown variables or noise) and errors of implementation (related to the oscillation of responses model coefficients when they are set on the machine or process) in the objective function [42];
iii) to use capability ratios where the variances of the models are taken as the components of natural variability, while the differences between the expected values and the nadir (worst) points are taken as the components of allowed variability [43];
iv) to consider the expectation and variance of the called squared error loss simultaneously [44];
v) to use a parameter-free solution ranking based on two concepts: an extended angle-based dominance technique from the algorithm called Adaptive angle-based pruning Algorithm (ADA) for discovering the knee solutions and the inverse-square law of light for enhancing the diversity of solutions [45];
vi) to use multiobjective evolutionary algorithms that iteratively updates a set of weight vectors to identify the Pareto optimal solutions that are close to reference points [46];
vii) to use multiobjective evolutionary algorithms that incorporate the DM's predefined target points within the region of interest on the Pareto front [47];
viii) to use multiobjective evolutionary algorithms that rank the optimal solutions based on their distance from ideal and anti-ideal solutions [48].

The list of previous cited papers is not exhaustive. The main concern in their selection was to present recent papers, published in relevant journals, that cite a collection of other papers that must be not ignored by those who use RSM and need to solve multiresponse problems.

2.1. Pareto solutions resilience

Multiresponse problems often involve the simultaneous minimization and/or maximization of k objectives, and can be formulated for the case of maximization as (1):

$$\text{maximize } \{f_1(\mathrm{x}), f_2(\mathrm{x}), \ldots, f_k(\mathrm{x})\}$$
$$\text{subject to: } \mathrm{x} \in \mathrm{X} \tag{1}$$

where $f_1(x), f_2(x), \ldots, f_k(x)$ are k objectives (functions or responses) to be maximized, x is the decision vector, and X is the set of feasible solutions. The most favourable solutions to these problems are, from a theoretical point of view, called nondominated or Pareto solutions. A decision vector x_1 ($\mathrm{x}_1 \in \mathrm{X}$) is said to Pareto dominate a decision vector x_2 ($\mathrm{x}_2 \in \mathrm{X}$), or by other words is nondominated, usually denoted as $\mathrm{x}_1 \succ \mathrm{x}_2$, if and only if

$$\begin{cases} f_i(\mathrm{x}_1) \geq f_i(\mathrm{x}_2), \text{for all } i \in \{1, 2, \ldots, k\} \\ f_i(\mathrm{x}_1) > f_i(\mathrm{x}_2) \text{ for at least one } i \in \{1, 2, \ldots, k\} \end{cases} \tag{2}$$

In multiresponse problems, where responses are usually in conflict, the number of Pareto solutions is typically large, which makes it difficult to select the best one to implement in the production process (equipments). Moreover, there is no guarantee that the values of future observed responses in the production process will be equal to the theoretical estimated responses due to the natural variability in the process, uncertainty associated with the estimated response values, truncation or rounding of the input variables value, reliability of the data collected, and other planning and technical errors [2,3]. Thus, assuming that the experiments were well planned and conducted, and their results appropriately analysed, a novel metric, the gradient norm, is used in this paper to assess and rank the nondominated solutions in terms of their resilience (sensitivity to truncation, rounding, and perturbations in the variables setting when implemented in the production process (equipments) or during its operation).

To better understand the impact of small changes (adjustment, variation, …) in variable settings over the solutions resilience, let's assume that Fig. 1 is a graphical representation of a univariate polynomial function $f(\mathrm{x})$. Solution x_2^* corresponds to a point in the response surface whose slope is lower than that of x_1^* so it will be more likely to achieve the $f(\mathrm{x}_2^*)$ value when solution x_2^* is implemented in the production process than the $f(\mathrm{x}_1^*)$ value by implementing solution x_1^*. In fact, if the same change (Δ) in x_1^* and x_2^* values occurs, one can see in Fig. 1 that $f(\mathrm{x}_1^* \pm \Delta)$ - $f(\mathrm{x}_1^*) \gg f(\mathrm{x}_2^* \pm \Delta) - f(\mathrm{x}_2^*)$, which means that solution x_2^* is more resilient or, by other words, its reproducibility is much higher than that of x_1^*.

In supplement to works that, in addition to bias, focus on the assessment of solutions' quality of prediction and solutions' robustness [34–36,44,49], this paper introduces a new metric for ranking the

resilience of Pareto solutions, the Gradient Norm [50,51]. This metric will aid the decision-maker in taking a more informed decision when he/she selects an optimal solution for solving a multiresponse problem. In practice, he/she can argue that a Pareto solution is more resilient than another one if the coordinates of the Pareto solution correspond to a point in the n-dimensional surface defined by $f(\mathrm{x})$ whose magnitude of the gradient at x (slope) is much lower than that of other solutions.

2.2. Gradient method

In optimization problems developed under the RSM framework, the function $f(\mathrm{x})$ or response is defined, in general, by a second order polynomial function whose graphical representation is a curved surface. The gradient of a scalar function $f(\mathrm{x})$ is a multidimensional derivative of that function, and it is represented by $\nabla f(\mathrm{x})$, called a vector field, where ∇ is called Nabla-Operator. For a n-dimensional scalar function $f(x_1, x_2, x_3, \ldots, x_n)$,

$$\nabla f(\mathrm{x}) = [\partial f(\mathrm{x}) / \partial x_1, \partial f(\mathrm{x}) / \partial x_2, \partial f(\mathrm{x}) / \partial x_3, \ldots, \partial f(\mathrm{x}) / \partial x_n] \tag{3}$$

The derivative of $f(x_1, x_2, \ldots, x_n)$ at each one of the directions $(x_1, x_2, \ldots, x_n)$ represents the slope in the response surface according to that direction (or spatial coordinate). Thus, as higher the slope of the surface is, as greater the gradient value will be. The maximum slope at x of a surface defined by $f(x_1, x_2, \ldots, x_n)$ is achieved by the gradient norm (4), and as higher the slope is, as greater the change in $f(\mathrm{x})$ value will be for a small increment or decrement in the settings of spatial coordinates $(x_1, x_2, \ldots, x_n)$.

$$\|\nabla f(\mathrm{x})\| = \sqrt{\left(\frac{\partial f(\mathrm{x})}{\partial x_1}\right)^2 + \left(\frac{\partial f(\mathrm{x})}{\partial x_2}\right)^2 + \ldots + \left(\frac{\partial f(\mathrm{x})}{\partial x_n}\right)^2} \tag{4}$$

In a multiresponse problem, the change in each response ($f(\mathrm{x})$) value due to small increment or decrement in the settings of $(x_1, x_2, \ldots, x_n)$ must be as small as possible in order to get the desired response's resilience. Note that response's resilience must be as high as possible to guarantee the expected reproducibility of the selected solution in the production process (equipments).

Pareto solutions are of special interest to the decision-maker for solving a multiresponse problem because, theoretically, they allow to achieve the best compromise among the responses. However, some Pareto solutions may not yield the expected value for one or more functions when implemented in production processes (equipments). This means that it will be useful to rank Pareto solutions in terms of their resilience. For this purpose, the metric suggested here is (4).

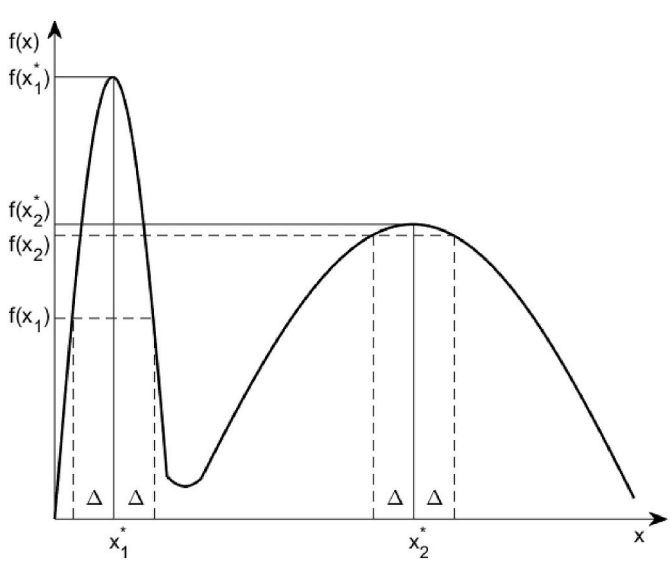

Fig. 1. Resilience of $f(\mathrm{x})$ solutions.

The most favourable Pareto solution is the one that, for all the k functions simultaneously, yields the smallest gradient norm value, i.e., has the highest resilience. However, this may not occur. In this case, solution selection process can be more problematic, requiring a compromise among responses whose priority may be not unequivocal. In practice, the decision process may include, among other decision-maker's options, the following one:

- Select the optimal solution achieved from (5),

$$rGN = min\left(\sum_i w_i \left(\left\|\nabla f_i\left(x_m^*\right)\right\| \Big/ max\|\nabla f_i(\mathrm{x})\|\right)\right) \tag{5}$$

where rGN stands for relative gradient norm, w_i is the weight or priority assigned by the decision-maker to the i-th response ($i = 1, 2, \ldots, k$), with $\sum_i w_i = 1$, x_m^* represents the variables setting of the m-th Pareto solution ($m = 1, 2, \ldots, p$), and $max\|\nabla f_i(\mathrm{x})\|$ is employed to normalize the responses values.

Note that solutions with high gradient norm value (low resilience) are not recommendable because this means that those solutions are highly sensitive to small changes in variables settings, namely due to truncation and rounding of the variable values required to implement them in the production process (equipments) or due to changes in their value during production process (equipments) operation. In practice, this implies that production process (equipments) behaviour or the characteristics of their output will be not the expected ones or, by other words, the theoretical value achieve for each response from data analysis will be not reproduced during production process (equipments) operation. To avoid it, and when weights or priorities are assigned to responses, the decision-maker must select the Pareto solution whose rGN value is the smallest one.

3. Results and discussion

To show the usefulness of the proposed metric, i.e., to assess the resilience of Pareto solutions, a classical case study was selected from the literature [1,25,52]. The study objective is to simultaneously optimize three responses in a chemical process: maximize the yield ($f_1(\mathrm{x})$), set viscosity ($f_2(\mathrm{x})$) on target, and minimize the molecular weight ($f_3(\mathrm{x})$). The controllable variables are the reaction time (x_1) and the reaction temperature (x_2). Experiments were run using a Central Composite Design, and the observed responses are shown in Table 1.

The models fitted to responses in coded variables, such as presented in [1, 25, 52] are

$$\widehat{f_1}(\mathrm{x}) = 79.94 + 0.995x_1 + 0.515x_2 + 0.250x_1x_2 - 1.376x_1^2 - 1.001x_2^2 \tag{6}$$

$$\widehat{f_2}(\mathrm{x}) = 70.00 - 0.155x_1 - 0.948x_2 - 1.250x_1x_2 - 0.688x_1^2 - 6.688x_2^2 \tag{7}$$

$$\widehat{f_3}(\mathrm{x}) = 3386.15 + 205.10x_1 + 177.35x_2 \tag{8}$$

and responses constraints are the following: $f_1(\mathrm{x}) \geq 78.5$; $62 \leq f_2(\mathrm{x}) \leq 68$ with target value equal to 65; $f_3(\mathrm{x}) \leq 3300$.

Figs. 2–4 show the response surface for each response separately, the range of response values, and the location of the Pareto solutions set. These figures also enables to visualize the range of operating conditions (x_i values) that produce the desired output for each response. The presented responses surfaces are not similar neither in shape nor in slope, which highlights the need of the gradient norm for assessing and selecting a solution for multiresponse problems. The overlaid of contour plots shown in Fig. 5 provides a visualization of the Pareto solution set location for the three responses and the range of x_i values. In this case, the Pareto set location is in a region delimited by $78.5 \leq \widehat{f_1}(\mathrm{x}) \leq 79.26$, $64.98 \leq \widehat{f_2}(\mathrm{x}) \leq 68$, and $3175.8 \leq \widehat{f_3}(\mathrm{x}) \leq 3284.30$.

Table 1
Experiments and Response values.

Natural Variables		Coded Variables		Responses		
Time (min)	Temperature (°F)	x_1	x_2	$f_1(x)$ (Yield)	$f_2(x)$ (Viscosity)	$f_3(x)$ (Molecular weight)
80	170	−1	−1	76.5	62	2940
90	170	1	−1	78.0	66	3680
80	180	−1	1	77.0	60	3470
90	180	1	1	79.5	59	3890
77.93	175	−1.414	0	75.6	71	3020
92.07	175	1.414	0	78.4	68	3360
85	167.93	0	−1.414	77.0	57	3150
85	182.07	0	1.414	78.5	58	3630
85	175	0	0	79.9	72	3480
85	175	0	0	80.3	69	3200
85	175	0	0	80.0	68	3410
85	175	0	0	79.7	70	3290
85	175	0	0	79.8	71	3500

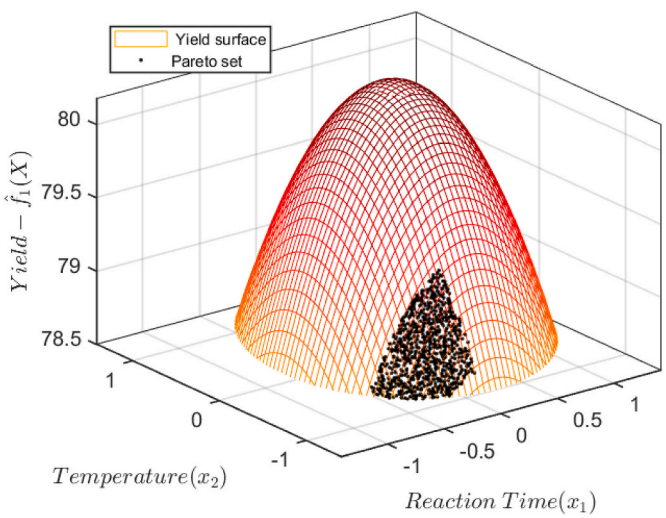

Fig. 2. Pareto solutions set and $\widehat{f_1}(x)$ response surface.

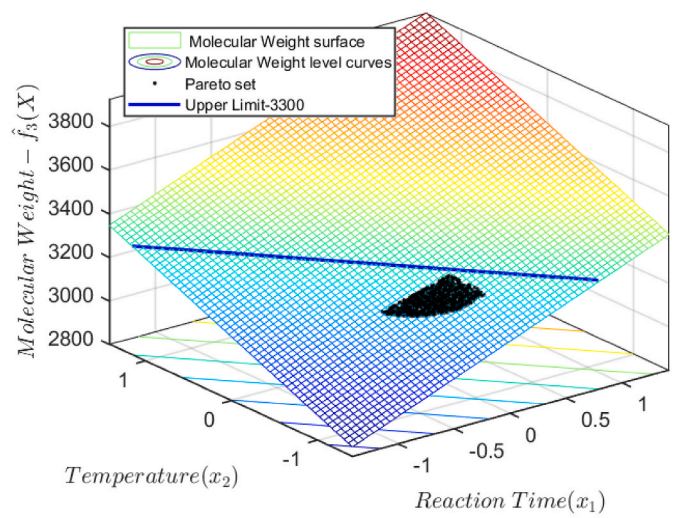

Fig. 4. Pareto solutions set and $\widehat{f_3}(x)$ response surface.

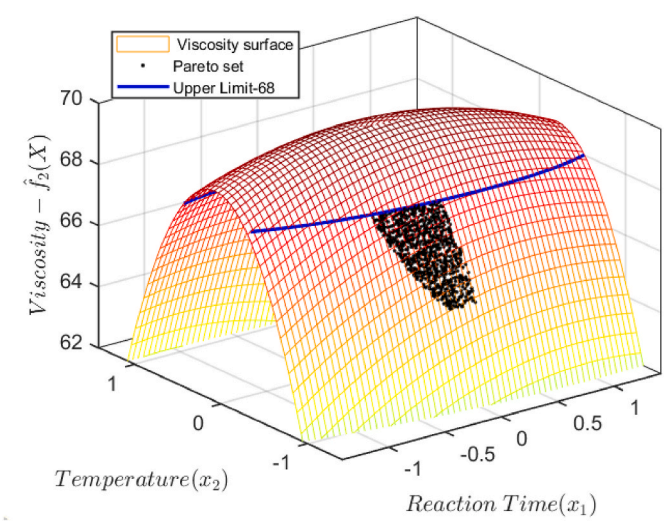

Fig. 3. Pareto solutions set and $\widehat{f_2}(x)$ response surface.

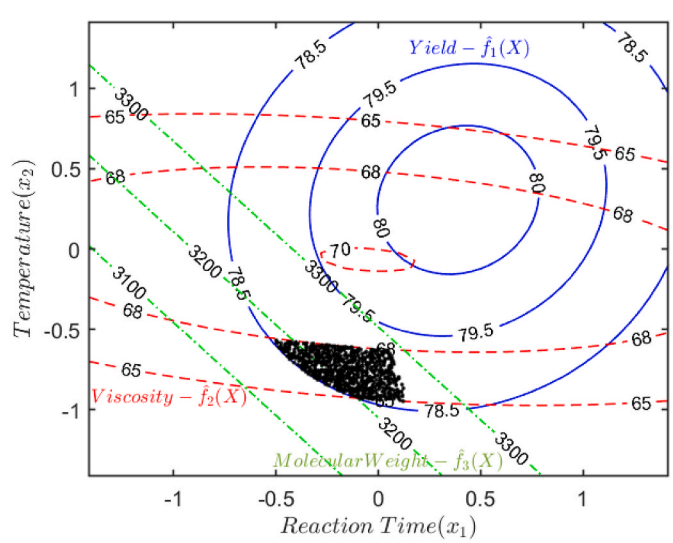

Fig. 5. Pareto solutions set and Overlaid Contour plot of responses.

The Pareto set represents the collection of solutions from where the solution for solving a multiresponse problem must be selected. However, Pareto solutions with a high gradient norm value should not be a priority choice because they will generate unexpected outputs due to truncation, rounding or changes in the input variables setting when implemented in production process (equipments) or during its operation, respectively. Figs. 6–8 show the gradient norm for each response and the respective range of x_i values, taking into account the constrains in the responses

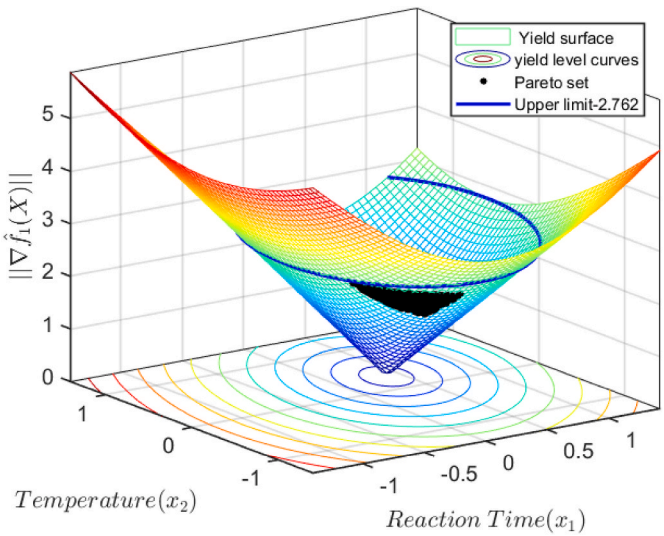

Fig. 6. Gradient norm surface for $\widehat{f_1}(x)$ and Pareto solutions set.

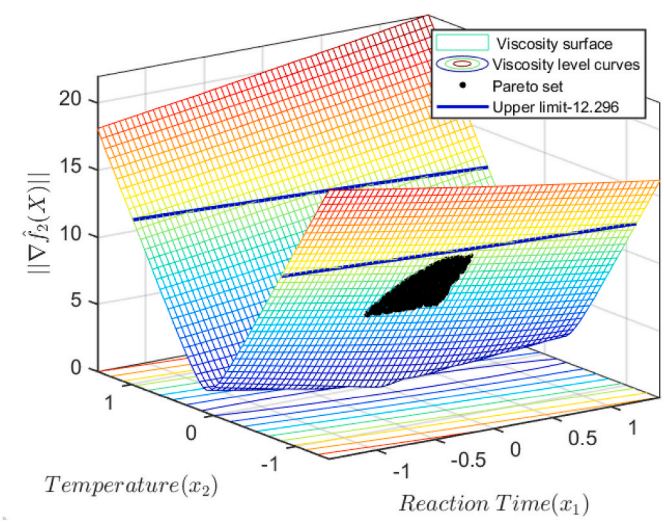

Fig. 7. Gradient norm surface for $\widehat{f_2}(x)$ and Pareto solutions set.

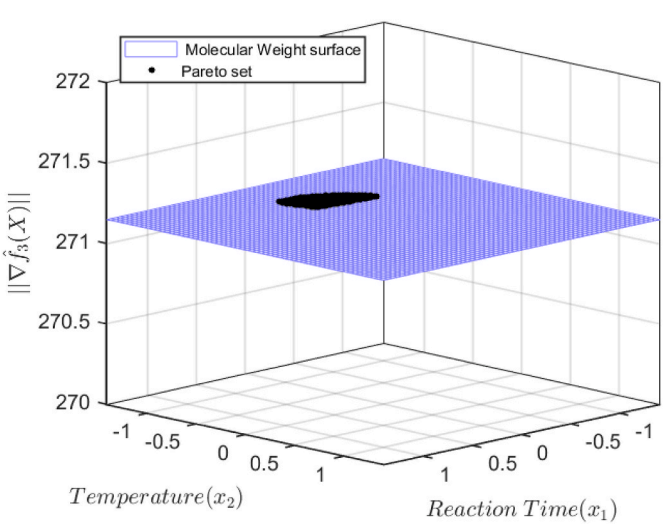

Fig. 8. Gradient norm surface for $\widehat{f_3}(x)$ and Pareto solutions set.

value, and include the maximum value (upper limit) of gradient norm value. In these figures it is apparent the different shape and magnitude of the gradient norm, which means that the gradient norm value of the Pareto solutions cannot be ignored in the solution selection process. The gradient norm value must be as low as possible to ensure that the selected solution has a resilence as high as possible to guarantee its reproducibility when implemented in production process (equipments) ou during its operation. It is important to highlight that to calculate the gradient norm value does not require from the data analyst a significant background in mathematics. This is an easy task because, for problems developed in the RSM framework, it consists in calculating derivatives of polynomial functions.

Fig. 9 shows Pareto solutions set delimited by the gradient norm values of each response, namely $1.922 \leq \|\nabla \widehat{f_1}(x)\| \leq 2.715$, $7.383 \leq \|\nabla \widehat{f_2}(x)\| \leq 11.668$, and $\|\nabla \widehat{f_3}(x)\| = 271.15$. These values show a variation in the functions gradient norm values approximately equal to 41% for $\widehat{f_1}(x)$ and 58% for $\widehat{f_2}(x)$, which means that the difference between theoretical and practical results for these responses can be significant. In this case study, the gradient norm value of $\widehat{f_3}(x)$ is constant, which simplified the solution selection. Nevertheless, to identify a Pareto solution whose gradient norm value is the smallest for all responses simultaneously, in order to guarantee the reproducibility of the theoretical responses values in the production process (equipments), it is not easy, if at all possible.

To select a solution from the Pareto set, the decision-maker may assign priorities to responses based on his/her preferences, namely technical and economical considerations, and taking into account the solutions reproducibility (the risk of responses value are very different from the theoretical ones) when implemented in production process (equipments) or during its operation. An approach to implement this procedure may consists in using the criterion (5). In this case, the decision-maker can test various combinations of w_i values and to identify a solution of higher resilience. The w_i values may depend on technical, economic, and other subjective decision-maker's preferences. Thus, when he/she is uncertain about the choice of w_i values, to decide without understanding the impact of these subjective choices is not recommendable, because it may lead to the selection of a solution with lower resilience.

Fig. 10 displays the Pareto solutions gradient norm values achieved from *rGN* (5), for all combinations of (w_1, w_2) values. As an example, for $(w_1, w_2) = (0.7, 0.3)$ the $rGN = 0.669$ whereas for $(w_1, w_2) = (0.2, 0.8)$ the $rGN = 0.623$. A similar solution selection procedure is applied if $\|\nabla$

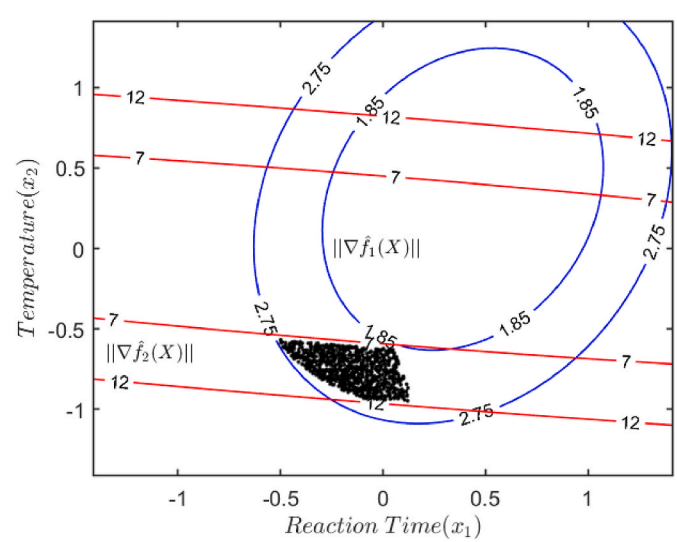

Fig. 9. Overlaid contour plot of gradient norm values and Pareto solutions set.

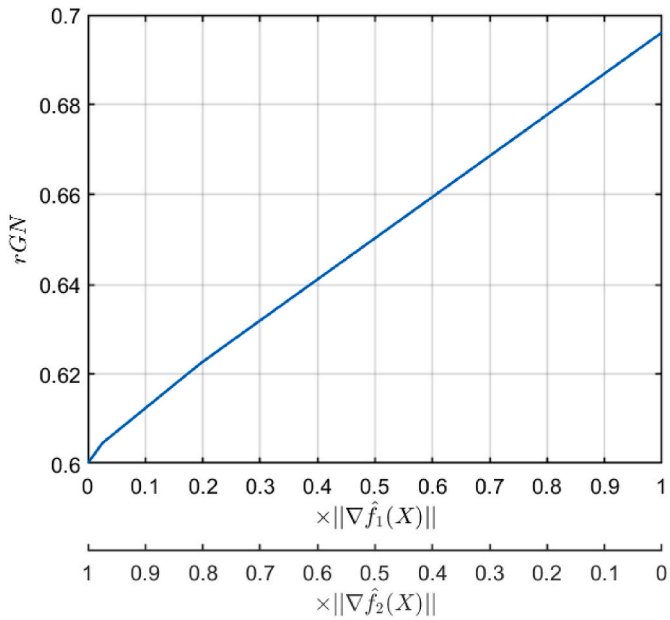

Fig. 10. *rGN* values.

$\widehat{f}_3(x)\|$ value was not constant, what occurs when a second or higher order model is fitted to this response. In this case a mixture (ternary) plot may be utilized for aiding in the decision-making process [25]. Other graphical representation may accommodate a high number of responses, such as shown in Ref. [22]. Nevertheless, it is important to note that when the number of responses increase, the computational burden to identify a representative set of Pareto solutions and the number of candidate solutions will increase substantially as well. In these cases, making effective comparisons between alternatives becomes more difficult. Consequently, it is important to carefully bound the number of responses to consider, without losing the ability to solve the problem. In these cases, though there are sophisticated approaches for Pareto solution visualization and evaluation, to facilitate the solutions ranking and the selection of a nondominated solution of decision-maker preference, a summary table will be appropriate. In fact, for more than three input variables, a summary table may provide the simplest summary of the results (variables settings, Pareto solutions, gradient norm values and other metrics of interest), and facilitate the solutions ranking and, consequently, the solution selection process. Regarding the calculus of the gradient norm values, this is a much more laborious task if responses modelling tools like Support Vector Machine and Gaussian Process regression are used instead of other like ordinary, partial, and generalized least squares.

4. Conclusions

This paper presents a new and easy-to-implement tool to select a solution from the Pareto solutions set. It can be applied by those who use responses aggregation indexes, as the popular desirability index, or any other method to generate solutions for multiresponse problems. Moreover, its application is not limited to problems developed in the RSM framework.

Solutions resilience has not been considered by researchers and practitioners so a metric to assess Pareto solutions resilience is proposed and its usefulness illustrated. This metric and the associated criterion for selecting a solution must be used by those who are engaged with multiresponse problems and want to avoid wasting resources and time in implementing theoretical solutions in production process (equipments) that do not produce the expected product or equipment behaviour.

Author statement

Nuno Costa: Conceptualization, Writing, Reviewing and Editing,
João Lourenço: Conceptualization, Writing, Reviewing and Editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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