Response Surface Optimization with Discrete Variables

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Recent advances in non-gradient based optimization methods (e.g., Genetic Algorithms, Particle Swarm Optimization) enhanced the abilities of discrete, integer, and mixed optimization problems. However, the very nature of non-gradient based algorithms is that the number of analyses required to get to an optimal solution is several orders of magnitude higher than for traditional gradient based optimization methods or response surface optimization methods, when considering continuous problems. Instead of these approaches we propose to use a response surface approximate optimization method modified to work with discrete design variables. In this case whenever it is required to perform the actual analysis of responses for the purpose of fitting a response surface approximation, the design variables will be converted to corresponding discrete values. Two discretization techniques are proposed. We demonstrate that although lacking global search properties like Genetic Algorithms and Particle Swarm Optimization, the discrete response surface optimization provides a computationally efficient way of improving an initial design and getting into a region of an optimum using only discrete points for analysis.

I. Introduction

Recent advances in such non-gradient based optimization methods like Genetic Algorithms [1] and Particle Swarm Optimization[2] definitely enhanced the abilities of discrete, integer, and mixed optimization problems. Non-gradient based methods provide a bigger chance of finding the global optimum during optimization and do not impose an extra penalty for performing discrete optimization when compared to performing continuous optimization. In fact, Genetic Algorithms are better suited for performing discrete than continuous optimization. So, use of non-gradient based optimization is a definite step forward in practical discrete optimization, when compared to such traditional methods like, for example Branch-and-Bound[3]. However, the very nature of non-gradient based algorithms is that the number of analyses required to get to an optimal solution is several orders of magnitude higher than for traditional gradient based optimization methods or response surface approximate optimization methods, when considering continuous problems. Also the very nature of these algorithms impose the practical limit of about a dozen design variables for a typical problem. Because of these reasons, the question arises of how to perform discrete optimization for practical problems when the time of performing a single analysis may be hours.

The easiest solution to this problem is to perform a continuous optimization using a gradient based or a response surface method and to round the optimum design variables to the nearest discrete values. However, this approach has a couple of well-known deficiencies: first of all, it is not necessary clear whether a particular variable should be rounded up or down, and it is not obvious a priori whether the obtained solution will satisfy all the specified design constraints. In addition, even if the obtained solution satisfies all the design constraints, the solution may not be optimum: a better solution may be available when skipping the closest discrete value for a particular design variable and going to the next one. Such a situation can occur for example, when optimizing the stacking sequence for composite laminates.

Instead of this approach, we propose to use a response surface approximate optimization method[4] modified to work with discrete design variables. In this case whenever it is required to perform the actual analysis of responses

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for the purpose of fitting a response surface approximation, the design variables will be converted to corresponding discrete values. Two ways of discretization are proposed. The first is a more traditional approach where the continuous values are rounded to the nearest discrete value. The second method is more elaborate. Because the response surface approximation is readily available, we may use the performance of the response surface approximation in the neighborhood of the continuous optimum as a guideline for finding the most favorable discrete point in the neighborhood of the continuous optimum. So that rounding will be performed not necessarily to the nearest value, but to the best discrete value in the neighborhood, according to the current approximation. IN addition, when we introduced the discretization of the design variables in the course of optimization, better results were obtained than simply rounding the design variables of the final continuous optimal solution to the discrete values.

The advantage of the proposed approach is that the number of required analyses, should be comparable to that of a continuous response surface approximate optimization of the same dimension. And this number is one or several orders of magnitude lower than the number of analyses required by non-gradient based optimization methods.

In this paper the results of using the two proposed approaches are compared to the best known discrete optimum and to the results of using a continuous gradient based optimization, when Branch-and-Bound method is applied after the continuous optimum is found.

II. Response Surface Methodology

A. Baseline Continuous Response Surface Methodology

A great variety of response surface methodologies is currently used in industry and academia. For our work we employed the methodology implemented in the VisualDOC software by Vanderplaats Research and Development, Inc.[5] In this methodology, the optimization process starts by selecting an initial design of experiments to fit the response surface to. Typically, to reduce computational cost, the initial design of experiments is selected to fit a linear polynomial response surface model. Examples of such design of experiments are a Koshal design[6] for a linear model and a Simplex design[6]. For our particular case we used a Simplex design. After the initial response surface approximation is constructed, a regular gradient based optimization is used to find an approximate optimum. At this stage the responses for the problem are evaluated using the responses surface approximation instead of the actual analysis. Once the approximate optimum point is found, an actual analysis is performed at this approximate optimum point. Using the analysis results, the response surface approximation is updated and a regular gradient based optimization is used to find a new approximate optimum. The procedure is repeated until the convergence criterion is satisfied. Thus, only one actual analysis is performed for each design iteration. One should notice that in this procedure the actual analyses are performed at points picked by the optimizer. These points do not necessarily have discrete values of the design variables.

B. Discrete Response Surface Methodology with Rounding

The goal of the present paper is to consider response surface methods that allow performing the analyses only for points that have discrete or integer values of the design variables. The easiest way to do that and to employ the response surface methodology described above is to round the discrete design variables at the approximate optimum point of each iteration to the nearest discrete value. After the design variables are rounded the analysis is performed and the new discrete point is added to the existing pool of analyzed design points. Using this pool of points the response surface approximation is recreated. The procedure is repeated for each iteration until the convergence criterion is satisfied.

As mentioned in the previous section, the response surface optimization process is started by performing an initial design of experiments to create the first response surface approximation. For the discrete response surface methodology with rounding these initial points should also be rounded to their closest discrete values to ensure that only discrete points are analyzed

C. Response Surface Methodology with Performance Based Discretization

The described methodology of rounding design variables is certainly one of the easiest and computationally efficient to convert the continuous values of design variables to discrete values. However, the obvious question arises whether this is the best approach of converting continuous design points to equivalent discrete design points in terms of getting the best optimization result.

One other way of converting continuous values to discrete ones is to make use of the current response surface approximation at each design iteration to select the best discrete optimum point. Of course, evaluating all the possible combinations of discrete values is computationally prohibitive even if we use the response surface approximation as the analysis. Moreover, when the number of discrete variables is relatively large (ten or more) it is computationally expensive to evaluate the approximate performance of the discrete points that directly “surround” the current continuous point. One may see that each discrete variable could be rounded up or down to the closest discrete value. Thus the number of all possible combinations to be evaluated is 2^n, where n is the number of discrete design variables.

To efficiently involve the response surface approximation performance into the discretization process, we decided to employ a method that is similar to the central finite difference technique in calculating the gradients. For a nominal continuous point we have to decide whether we should round each discrete design variable up or down. When rounding to the closest discrete point it is possible to make this selection based on the coordinates of the continuous point and on the corresponding discrete values. In the alternative approach that we propose we want to make this selection (whether to round up or down) based on the performance of the response surface approximation.

The process of selecting the discrete value to which the nominal continuous point will be rounded in the proposed approach is as follows. One discrete variable of the continuous nominal point is at first rounded up. The performance of the obtained point is evaluated using the response surface approximation: the approximate values of the objective function and constraints are evaluated. Next, the same discrete variable is rounded down. Again the performance of the obtained point is evaluated using the response surface approximation. The performance of the two rounded points is compared to determine if the particular variable should be rounded up or down. This procedure is repeated separately for each discrete variable. Finally, the obtained discrete point is analyzed and added to the existing pool of analyzed points. The response surface approximation at the next design iteration is created using this updated pool of analyzed design points.

III. Results

We used several example problems to evaluate the performance of the proposed approaches. The results from the proposed approaches were compared with the known optimal solutions and with the results of the continuous gradient based optimization, when Branch-and-Bound method was applied after the continuous optimum was found.. The sequential quadratic programming method (SQP) was used as a continuous optimization method.

A. Rounded Box Example Problem

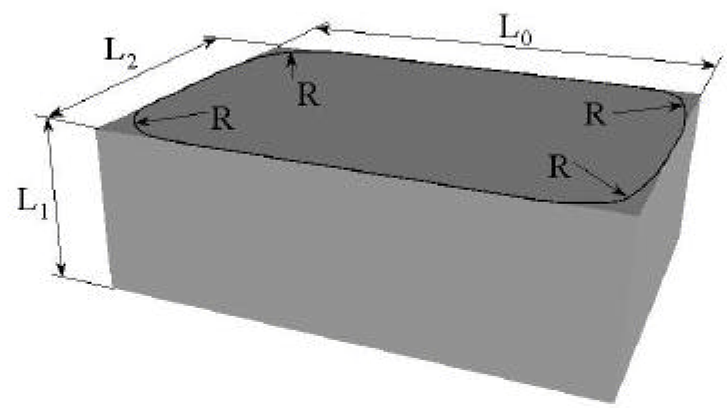

Figure 1: Rounded Box.

Figure 1 shows the rounded box. The optimization problem was formulated to find the minimum volume of the box such that the surface area of the box would be within certain bounds. The dimensions of the box (L_0, L_1, L_2, R) were the design variables. The design variables L_0, L_1, L_2 were allowed to assume only one of the following values: 30, 35, 40, 45, 50. The radius of the corners (R) was allowed to take the values of 10, 15, 20. The surface area was restricted to be within the bounds of [6,000 to 10,000].

Table 1 below summarizes the results produced by both discrete response surface approaches, by the SQP optimization followed by the Branch-and-Bound method, and the true optimum found by simply looking at all possible combinations.

One can see that both discrete response surface optimization methods got relatively close to the true optimum, while the SQP followed by the Branch-and-Bound found the exact optimum. The number of analyses required by the SQP followed by the Branch-and-Bound approach is more than an order of magnitude higher than that of two discrete response surface approaches. Note that all the methods started optimization from an infeasible design.

Parameter	**Initial**	**Rounding to Closest**	**Performance Discretization**	**SQP**	**Exact**
L_0	50	30	30	30	30
L_1	50	50	50	30	30
L_2	50	30	30	45	45
R	10	15	15	15	15
Volume	120,708	35,343	35,343	34,706	34,706
Surface Area	13,970	6,126	6,126	6,041	6,041
# of analyses		8	9	381	

Table 1: Results of the Rounded Box Problem

B. Lap-Joint Example Problem

Figure 2 shows the two plates joined together by three rows of rivets. The plates are pulled apart. The optimization problem was formulated to find the minimum number of rivets that will satisfy the shear stress constraints. The diameter of rivets is allowed to take only specified discrete values (the same diameter is used for all rivets).

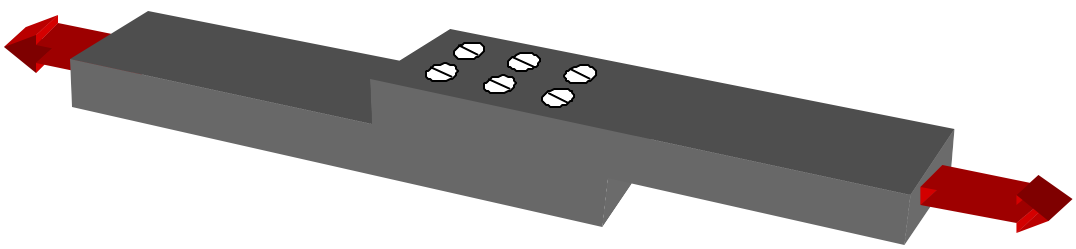

Figure 2: Riveted Lap-Joint.

Table 2 below summarizes the results produced by both discrete response surface approaches, by the SQP optimization followed by the Branch-and-Bound method, and the true optimum found by examining all possible combinations. In this table N_1 is the number of rivets in the first row, N_2 is the number of rivets in the second row, N_3 is the number of rivets in the third row, d is the diameter of the rivets.

This particular problem has many solutions with the characteristics of the exact optimum, because many combinations of design variables could produce the relatively large surface of rivets to avoid failure in shear.

One can see that here the response surface method involving rounding to the closest discrete point failed to find a feasible solution. Whereas the performance based response surface discretization and SQP followed by the Branch-and-Bound both found the exact optimum. In this example problem once again the number of analyses required by the SQP followed by the Branch-and-Bound approach is significantly higher than that of two discrete response surface approaches. Note that all the methods started optimization from an infeasible design.

Parameter	**Initial**	**Rounding to Closest**	**Performance Discretization**	**SQP**
N_1	5	9	11	9
N_2	5	14	12	15
N_3	5	7	16	15
d	0.01	0.02	0.02	0.02
N total	15	27	39	39
Feasible?	*infeasible*	*infeasible*	feasible	feasible
# of analyses		16	29	167

Table 2: Results of the Lap-Loint Problem

C. Other Examples

In addition to the examples described above we evaluated the performance of the considered approaches on a number of other examples. For the majority of the examples considered the performance based discretization approach was consistently outperforming rounding to the closest discrete values.

However, it should be noted that we were not able to solve all test problems using the approaches considered. One such problem is a cantilevered stepped beam problem briefly described below.

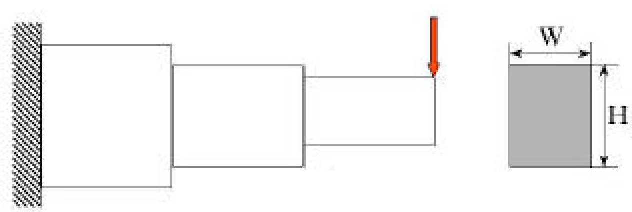

Figure 3: Cantilevered Stepped Beam.

Figure 3 shows the configuration of the stepped beam. The number of segments in the beam is fixed. The length of each segment is also fixed. The design variables are the height (H) and width (W) of each segment. The height of the beam should be not more than 20 times the width of the beam to preserve a reasonable configuration. The objective is to minimize the volume of the beam while satisfying bending stress constraints and maximum tip deflection constraint. We used the problem setting with five segments. Thus 10 discrete design variables were used (five for widths and five for heights of individual segments).

This problem in general was found to be difficult for the responses surface methodology to solve. Even when all the design variables used were continuous. When discretization was added on top of the response surface methodology, none of the considered approaches was able to find a feasible optimal solution or get reasonably close to it. This shows that the discretization imposed on top of the response surface methodology may worsen the performance of the responses surface optimization, if some special precautions are not taken.

IV. Conclusions

One should realize that the results obtained in this paper are closely related to the baseline response surface methodology used. However, we believe that if a different implementation of the response surface optimization is used the general trends could be similar to what we discovered.

Two discretization approaches were proposed for usage along with the responses surface methodology. The approaches were compared with each other and with a gradient based optimization followed by the Branch-and-Bound method. The performance based discretization approach consistently produced better optimization results in our test cases. This leads to a suggestions of employing the performance of the response surface approximation for the discretization procedure whenever available.

Performance of the discrete response surface optimization exhibits the same drawbacks as that of the continuous responses surface optimization: relatively low number of design variables (up to 20 or so), etc. In addition, the discretization seems to worsen the response surface optimization performance.

Although lacking global search properties like Genetic Algorithms and Particle Swarm Optimization, the discrete response surface optimization provides a computationally efficient way of improving an initial design and getting into a region of an optimum using only discrete points for analysis.

In the future we may concentrate the research related to this topic in the area of improving the performance of the response surface optimization procedure for the case of relatively large numbers of discrete design variables. This may include improving the performance of the baseline response surface methodology. Also we may investigate some special precautions that could lessen the negative effect that discretization has on the response surface optimization procedure.

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