RESPONSE SURFACE AND SENSITIVITY-BASED OPTIMIZATION IN LS-OPT: A BENCHMARK STUDY

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Abstract

This paper evaluates the robustness of LS-OPT for response surface and design sensitivity-based optimization. The methodology uses linear response surfaces constructed in a subregion of the design space. These are constructed using either a design of experiments approach with a *D*-optimal experimental design or the available analytical or numerical gradient. The approach utilizes a domain reduction scheme to converge to an optimum. The scheme requires only one user-defined parameter, namely the size of the initial subregion. To test its robustness, the results using the method are compared to SQP results of a selection of the well-known Hock and Schittkowski problems. Although convergence to a small tolerance is predictably slow when compared to SQP, LS-OPT does remarkably well for these, sometimes pathological, analytical problems.

Introduction

The success of finite element simulation to augment or even replace physical experimentation in design has accelerated the development of simulation-based optimization in recent years. While having its origins in the statistics of physical experimentation, response surface methodology (RSM) (Box & Wilson, 1951, Myers and Montgomery, 1995) has been the primary gradient-free simulation-based approach available. The general unavailability of analytical gradient information in analysis codes arises from the complexity of the non-linear finite element formulation. While not requiring any code enhancement, an alternative approach by means of finite differences may result in spurious gradients, not suitable for gradient-based optimization. For these reasons, and because of the noise-filtering properties of RSM, it has become particularly popular for impact design applications such as crashworthiness or metal forming where the response can be highly nonlinear.

As analysis methods for impact dynamics began to take hold in industry in the late eighties, design optimization methods of impact design followed in the mid 1990's. Among the topics studied are occupant safety (Etman *et al*, 1996, Etman, 1997), component-level optimization (Marklund, 1999, Akkerman *et al*, 2000), airbag-related parameter identification (Stander, 2000) and full-vehicle simulation (Sobieszczanski-Sobieski et al, 2000). The response surface method appeared in several forms, e.g. a successive response surface method (Toropov, 1989, Etman *et* *al*, 1996, Kok & Stander, 1999, Stander, 2001) and an updated response surface method (Schramm & Thomas, 1998, Sobieszczanski-Sobieski *et al*, 2000). Toropov (1989) experimented with linear and multiplicative approximations for his iterative multipoint approximation method and applied weighted least squares fitting and reduction of the subregion size based on function accuracy. In later work, Toropov presented refinements of his method in the form of indicators for move limit strategies. These criteria have been incorporated in a multipoint approximation strategy known as MARS (Toropov, 1998). The methodology of Etman (1997) uses a successive linear approximation approach with a saturated experimental design ($n + 1$ points, with n the number of design variables) within a subregion of the design space. To determine the location and size of each new subregion, a complex heuristic is used, based on oscillation, the accuracy of the response surface and constraint activity. More recently, Sobieszczanski-Sobieski et al (2000) conducted a full-vehicle simulation of a multidisciplinary nature while using a single set of higher-order response surfaces. In a metal-forming application Kok & Stander (1999) used a successive linear response surface method while Akkerman *et al* (2000) demonstrated the use of a similar but slightly enhanced successive approximation method to a knee bolster design with shape variables and involving transient mesh adaptivity.

While these studies demonstrate optimization capability by means of examples, there appears to be a dearth of benchmark studies that assess convergence properties of response surface-based methods. Against this background, the present paper reports on the robustness of the present LS-OPT (LSTC, 1999) methodology when applied to a large set of algebraic test problems. In addition, for these problems, the response surface approach is compared to the more standard Successive Linear Programming method (using design sensitivities) where both use the same adaptive domain reduction approach.

The motivation for the method proposed in the paper is derived from the requirements for simulation-based optimization (Craig & Stander, 2001):

1. *Robustness and accuracy*. In practical applications, it is important that the optimization method produces an answer to engineering accuracy or at least an immediate and significant improvement of the objective.
2. *Efficiency*. The number of expensive simulation-based function evaluations required for each design iteration must be limited. Direct optimization methods without approximations or evolutionary algorithms like the genetic algorithm are usually disqualified due to the large number of function evaluations required.
3. *Parallelization*. To improve efficiency, modern simulations run on multiple computers and/or processors. The optimization method must therefore be parallelizable. This disqualifies e.g. sequential line searches.
4. *Noise*. The step-size dilemma of gradient-based methods must be addressed as this impacts both robustness and efficiency. A noise filtering capability may avoid local optima.
5. *Infeasibility*. The algorithm must be able to start from and handle intermediate infeasible designs if they can be simulated. It must also be able to provide a best compromised design if no feasible design is possible within the constraints specified.
6. *Multidisciplinary optimization.* The method is required to interface to both response surfaces and design sensitivities (analytical and numerical).
7. *Global optimum.* This requirement is probably the strictest of all those listed. If an algorithm has features that at least provide the possibility of not terminating on the first

local optimum it finds, then this will be desirable in practical applications. The study of true global optimization algorithms lies outside the scope of this paper.

8. *Ease of use.* The number of user-selected parameters must be kept to a minimum.

A methodology that successfully addresses most of these requirements involves the following main components:

- Response Surface Methodology (RSM)
- Design Sensitivity Analysis (DSA)
- A Domain Reduction Scheme (Stander & Craig, 2002)

These strategies have been incorporated into a single algorithm capable of handling experimental design results as well as sensitivities.

The RSM (Myers & Montgomery, 1995) capability in LS-OPT involves a Design of Experiments approach to construct linear response surfaces on a subregion from a *D*-optimal subset of experiments. Linear functions are used to minimize the number of simulations required, especially for a very large number of variables. The size of each successive subregion is adapted based on contraction and panning parameters designed to alleviate oscillation and prevent premature convergence (Stander & Craig, 2002). To prevent remote designs from affecting the accuracy of the subregional optimum, simulation results from previous iterations are not incorporated and each response surface is strictly based on the results of a *D*-optimal experimental design within the current subregion. The method handles noisy responses automatically through the selection of an initially large subregion and a typically 50% over-sampling of experiments in the implementation of the *D*-optimality criterion (Roux, Stander & Haftka, 1998). As the optimum is approached, the subregion is contracted automatically, implying that inaccuracies in the sensitivity information do not cause large departures from the previous design. Therefore this handling of the *step-size dilemma* (Haftka & Gürdal, 1990) also provides an inherent move limit to the algorithm. The use of an adaptive subregion or trust region is not new, e.g., in Lin *et al* (2000), Pérez *et al* (2000), and Alexandrov *et al* (1997), the ratio of the simulated (actual) objective function reduction to that of the approximated objective function reduction in each design step is used as a measure to adjust the trust region size.

The SRSM method has proved itself to be robust but only moderately efficient if convergence to a tight tolerance is required. The over-sampling required for each response surface, although fully parallelizable, implies that it requires 50% more function evaluations for each design iteration than the minimum required by gradient-based algorithms using numerical gradients.

To incorporate gradient information within the given framework, a linear surface is fitted to the gradient at the design point. This conforms exactly to what is known as the SLP (Successive Linear Programming) method (see e.g. Arora, 1989).

Optimization codes are often applied in a multidisciplinary context (Craig *et al,* 2002) and therefore require the incorporation of both function values and gradients in the same optimization algorithm. The aim of the study is to illustrate that the proposed methodology can efficiently and robustly address both smooth (e.g. static or modal analysis) and noisy (e.g. crashworthiness) simulation-based problems. The test cases are randomly collected analytical and sometimes pathological problems from Hock & Schittkowski (1981) and are often used for testing optimization algorithms. These examples possess reliable gradient information, so one would expect a good local approximation method to also perform well. A crashworthiness/NVH design optimization problem will be presented at the conference to illustrate application of the method in a multidisciplinary setting.

Methodology of Successive Response Surface Method (SRSM)

Consider the general nonlinear optimization problem:

$$\text{Minimize } f(\boldsymbol{x}),\ \boldsymbol{x} \in R^n \tag{1}$$

subject to the inequality constraints

$$L_j \leq g_j(\boldsymbol{x}) \leq U_j; \quad j = 1,2,\ldots,m \tag{2}$$

and simple bounds on the design variables

$$x_{il} \leq x_i \leq x_{iu}; \quad i = 1,\ldots,n \tag{3}$$

where L_j and U_j refer to the upper and lower bounds on each of the inequality constraints, and x_{il} and x_{iu} the lower and upper bounds on each of the design variables, n is the number of design variables, and m the number of inequality constraints. Note that equality constraints can be written as two inequality constraints in the form of Equation 2 with L_j equal to U_j.

Refer to Roux, Stander & Haftka (1998) and Stander (2001) for a detail description of the Successive Response Surface Method (SRSM). The method, as implemented in LS-OPT (Stander, 1999), has a number of features that makes it robust and suitable for the solution of practical problems:

- The *D*-optimal experimental design is used to best utilize the number of available runs. Over-sampling of 50% is used to maximize the predictive capability (Roux, Stander & Haftka, 1998) of the response surfaces.
- Linear approximations are constructed using linear regression on all the points of the current iteration. Unit weighting is used for the regression. For gradient-based problems, a linear approximation is fitted to the gradient at the design point.
- An adaptive domain reduction method is applied as described in detail below.
- An auxiliary problem that minimizes the maximum constraint violation is solved to enforce feasible designs.

The SRSM method uses a region of interest, a subspace of the design space, to determine an approximate optimum. A range is chosen for each variable to determine its initial size. A new region of interest centers on each successive optimum. Progress is made by moving the center of the region of interest as well as reducing its size. Figure 1 shows the possible adaptation of the subregion. Details of the method are discussed in Stander, 2001 and Stander & Craig, 2002.

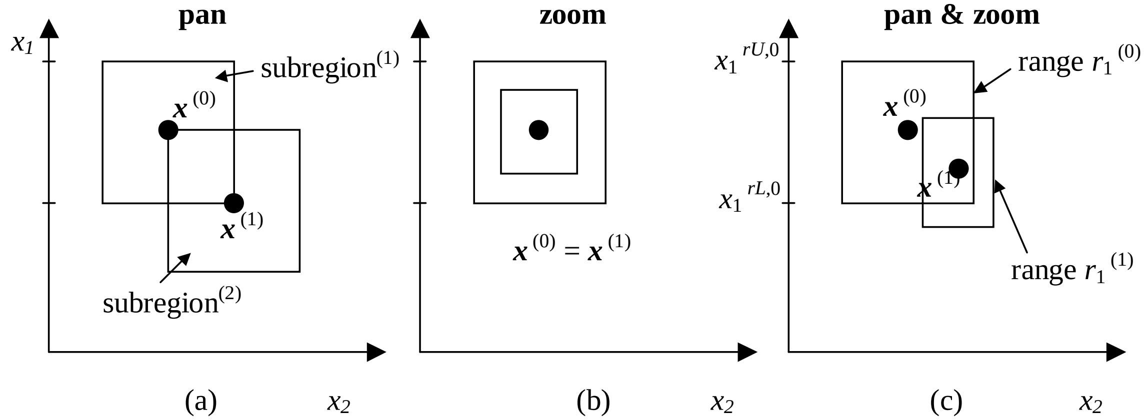

Figure 1 – Adaptation of subregion: (a) pure panning, (b) pure zooming and (c) a combination of panning and zooming

Test cases: Hock and Schittkowski problems

37 arbitrarily selected Hock problems and one problem from Svanberg (1995, 1999) are used in this benchmark with the same starting designs being used for testing all the algorithms. The problems are all analytical expressions with analytical gradients but the gradients are computed numerically to emulate a simulation-based environment to align the test with the thrust of this paper. Five of the problems (Nos. 2, 15, 16, 17, 20) are variations of the Rosenbrock problem ($f = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$), while the number of design variables ranges between 2 and 21. All the selected problems are constrained optimization problems.

Results and discussion

The results for the 38 problems are summarized in Tables I and II (see also Stander & Craig, 2002). The results obtained using Powell's Sequential Quadratic Programming (SQP) method as reported by Hock and Schittkowski are given in Table I, while the results for the SRSM and SLP method are given in Table II. *n* is the number of design variables.

Convergence is defined in terms of the objective function, with the number of iterations required for 1% and 0.01% convergence given in Tables I and II. The error on the objective is defined as

$$f_{err} = \frac{\left| f_{act} - f^* \right|}{1 + \left| f_{act} \right|} \times 100\% \tag{13}$$

where f_{act} is the exact objective function value (Hock, 1981) and f^* is the computed optimum.

For the SQP results, only final convergence values are available, and the iterations to this final value and the error are given. Note that, for each iteration, the objective function, constraint function(s) (if present) and their gradients must be evaluated. SRSM employs 1.5(*n* + 1) + 1 *D*-optimal design points for each iteration, while the SLP method uses a small finite-difference step size (10^{-6}), therefore requiring only *n* + 1 evaluations for the numerical gradient. For all the problems, unless otherwise indicated, the original subregion is 25% of the design space in each variable. No problems other than those reported here were attempted.

Problem #	n	f_{act}	SQP		
			f^*	Niter	f_{err}
2	2	0.0504	28.4	-	-
10	2	-1	-1	12	5e-8
12	2	-30	-30	12	1e-8
13	2	1	1	45	5e-8
14	2	1.39	1.39	6	8e-9
15	2	307	307	5	1e-8
16	2	0.25	23.1^+	-	-
17	2	1	1	12	1e-8
20	2	38.2	38.2	20	5e-9
22	2	1	1	9	1e-8
23	2	9	9	7	1e-8
24	2	-1	-1	5	1e-8
26	3	0	0	19	4e-8
27	3	0.04	0. 04	25	2e-8
28	3	0	0	5	3e-21
29	3	-22.6	-22.6	13	9e-11
30	3	1	1	14	1e-8
31	3	6	6	10	1e-8
32	3	1	1	3	1e-8
33	3	-4.59	-4^+	-	-
36	3	-3300	-3300	4	1e-8
45	5	1	1	8	1e-8
52	5	5.33	5.33	8	6e-9
56	7	-3.46	-3.46	11	1e-8
60	3	0.0326	0.0326	9	3e-8
61	3	-144	-144	10	2e-8
63	3	$952^{¥}$	962^+	-	-
65	3	0.954	2.8	-	-
71	4	17.0	17.0	5	2e-8
72	4	728	728	35	1e-8
76	4	-4.68	-4.68	6	3e-9
78	5	-2.92	-2.92	9	3e-9
80	5	0.0539	0.0539	7	8e-10
81	5	0.0539	0.0539	8	2e-9
104	8	3.95	3.95	19	8e-9
106	8	7050	7050	44	1e-5
108	9	-0.866	-0.697^+	-	-
12-corner polytope#	21	280	280	150	1e-6

Table I – Hock and Schittkowski problems (SQP): number of iterations Niter corresponding to objective f^* (error f_{err} and known optimum f_{act})

¥ SRSM found a lower optimum than that listed in Hock & Schittkowski (1981)

+ Converged to local optimum # Obtained by MMA (Svanberg 1995, 1999), not SQP

Problem #	n	f_{act}	Response Surfaces (SRSM)			Sensitivities (SLP)		
			f^*	Niter (1%)	Niter (0.01%)	f^*	Niter (1%)	Niter (0.01%)
2	2	0.0504	6.55	-	-	0.524	-	-
10	2	-1	-1	13	18	-1	24	27
12	2	-30	-30	5	11	-30	5	7
13	2	1	0.76	-	-	0.781	-	-
14	2	1.39	1.39	9	13	1.39	4	5
15	2	307	360+	-	-	306	5	-
16	2	0.25	0.25$	68	79	23.1+	-	-
17	2	1	1	8	11	1	6	6
20	2	38.2	40.2+	-	-	40.2+	-	-
22	2	1	1	8	12	1	5	5
23	2	9	9	13	18	9	1	2
24	2	-1	-1	2	2	-1	2	2
26	3	0	0	15	22	0	9	11
27	3	0.04	0.079	-	-	0.072	-	-
28	3	0	0	10	14	0	11	12
29	3	-22.6	-22.6	7	16	-22.6	5	9
30	3	1	1	9	10	1	9	12
31	3	6	6	8	15	6	8	11
32	3	1	1	1	1	1	2	2
33	3	-4.59	-4.59	4	9	-4+	-	-
36	3	-3300	-3300	5	5	-3300	5	5
45	5	1	1	6	6	1	6	6
52	5	5.33	5.33	9	15	5.33	6	11
56	7	-3.46	-3.46	15	25	-3.46	10	12
60	3	0.0326	0.0326	11	15	0.0326	11	23
61	3	-144	-144	6	11	-144	4	6
63	3	952¥	952	2	8	962+	-	-
65	3	0.954	0.954	18	22	0.954	14	16
71	4	17.0	17.0	4	10	17.0	2	5
72	4	728	728	34	53	820+	-	-
76	4	-4.68	-4.68	5	13	-4.68	3	8
78	5	-2.92	-2.92	20	28	-2.92	9	12
80	5	0.0539	0.0539	7	11	0.0539	1	6
81	5	0.0539	0.079	-	-	0.0539	4	6
104	8	3.95	3.95	8	14	3.95	8	18
106	8	7050	7050	8	13	7049	4	5
108	9	-0.866	-0.866	27	32	-0.675+	-	-
12-corner polytope	21	280	279	7	-	280	7	8

Table II – Hock and Schittkowski problems: number of iterations (Niter) corresponding to objective f^* (SRSM and SLP)

$ $\gamma_{pan} = 1.2$ + Converged to local optimum

¥ SRSM found a lower optimum than that listed in Hock & Schittkowski (1981)

The result of the twelve-corner polytope problem of Svanberg (1995, 1999) is also given in Tables I and II. Svanberg listed the optimum as 280, found in about 150 iterations (50 outer with about 3 inner iterations each) to an accuracy of 10^{-6} using the Method of Moving Asymptotes

(MMA) algorithm. Astonishingly, the SLP method finds this optimum to within 10^{-2} in 7 and to within 10^{-4} in 8 iterations.

Summary of tabled results:

- The SQP method fails to find a local minimum in 2 of the 37 problems it was tested on.
- The SRSM method fails to find a local minimum in 5 of the 38 problems with modification to the default heuristics only required once for convergence.
- The SLP method fails to find a local minimum in 4 of the 38 problems.

For three of the problems where SQP and SLP failed to converge to the global optimum (Problems 16, 33, and 63), SRSM performed better. E.g. for Problem 16, SRSM found the optimum in 80 iterations, but only through the alteration of γ_{pan} (see Stander & Craig, 2002) from the default value of 1.0 to 1.2. This is the only such amendment in this study. The SQP method, on the other hand, found the global optimum in Problems 13 and 20, while SRSM and SLP converged to local minima. Both SQP and SLP found the correct optimum in Problem 15, while SRSM converged to a local minimum. It should be emphasized that the results presented are for a single starting design for each problem, and that the ability of some of the algorithms to find the global optimum whilst others found local optima, is based on chance.

Remarks and Conclusions

A Successive Response Surface Method (SRSM) has been adapted to incorporate gradient-based optimization and was subjected to a variety of standard test problems.

The following conclusions can be drawn:

1. The SRSM method performed surprisingly well on the analytical test problems, even though it only used linear approximations. Convergence was in general slower than for SQP, but the contracting subregion helped the algorithm to move into close proximity of the optimum. In general, progress to the region of the optimum is rapid, followed by an expected slow convergence to a higher accuracy.
2. An SLP algorithm based on the same domain reduction scheme as SRSM proved to be successful for coarse convergence although it is expected to be successful only for smooth analytical problems.

Finally, the results in this paper demonstrate that, when considering coarse convergence properties, the performance of the Successive Response Surface Method does not differ dramatically from other, more established algorithms such as SQP. While the failure of numerical gradient-based methods such as SQP is well documented for noisy problems, it has been shown in the current paper and previous LS-OPT literature that SRSM has the potential of obtaining, with a reasonable degree of accuracy and without experimentation with user-selected parameters, converged optimization solutions to both smooth and noisy problems. This makes the algorithm ideal for multidisciplinary optimization problems in which multi-point approximations are suitably constructed for noisy functions (e.g. from crash simulations) and analytical gradients are available for smooth functions (e.g. modal frequencies).

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