

## ADAPTIVE EXPERIMENTAL DESIGN FOR CONSTRUCTION OF RESPONSE SURFACE APPROXIMATIONS.

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### Abstract

Sequential Approximate Optimization (SAO) is a class of methods available for the multidisciplinary design optimization (MDO) of complex systems that are composed of several disciplines coupled together. One of the approaches used for SAO, is based on a quadratic response surface approximation, where zero and first order information are required. In these methods, designers must generate and query a database of order  $O(n^2)$  in order to compute the second order terms of the quadratic response surface approximation. As the number of design variables grows, the computational cost of generating the required database becomes a concern. In this paper, we present a new approach in which we require just  $O(n)$  parameters for constructing a second order approximation. This is accomplished by transforming the matrix of second order terms into the canonical form. The method periodically requires an order  $O(n^2)$  update of the second order approximation to maintain accuracy.

Results show that the proposed approach is practical and convenient for engineering design problems by dramatically reducing the total number of calls to the simulation tools.

### Nomenclature

$f$	Objective function
$\mathbf{g}$	Inequality constraint vector
$g_i$	$i^{\text{th}}$ inequality constraint
$\mathbf{x}$	Vector of design variables
$\mathbf{x}_0$	Current design point
$f_0$	$f(x_0)$
$\mathbf{g}_0$	Vector of constraints $g_i(x_0)$
$\mathbf{H}(\cdot)_0$	Hessian matrix of $(\cdot)$ constructed around $x_0$
$\lambda$	Vector of Lagrange multipliers
$\Phi$	Augmented Lagrangian function

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### 1 Introduction

Applying nonlinear optimization strategies directly to complex multidisciplinary systems can be prohibitive when the complexity of the simulation codes is large. Increasingly, Response Surface Approximations (RSAs)

are being integrated with nonlinear optimizers in order to reduce the CPU time required for the optimization of complex multidisciplinary systems. RSAs provide a computationally inexpensive lower fidelity representation of the system performance space.

Two trends have emerged when integrating RSAs within nonlinear optimization tools: 1.) The use of global approximations where a RSA of the entire design space is developed and 2.) The use of local approximations, where RSAs are built within a local region around the current design. In general a single optimization is performed when employing global approximations. The cost of developing a good global response surface is obviously higher than for local responses as a more complex model is required to mimic the system. When using local response surfaces, a Sequential Approximate Optimization (SAO) methodology can be used. In SAO the design space is sampled around each design iterate to generate the data base required for constructing a low order polynomial using regression analysis (Box and Draper, 1987).

The authors have investigated two different approaches for design sampling in SAO frameworks. The first is an optimization based sampling, which has roots in the original Concurrent SubSpace Optimization (CSSO) algorithm of Sobieszczanski-Sobieski (1988). It was later modified for response surface approximate optimization in Renaud and Gabriele (1993, 1994), Wujek et al. (1997) and expanded to a formal framework for trust region model management in Rodríguez et al. (1998b). In this approach, each of the disciplines perform an optimization subject to move limits. The required inputs from other systems are computed by linear approximations. The design points visited through the subspace optimizations are stored and serve as the database for the RSA construction. The other approach, is a statistically based sampling using Design of Experiments (DOE) arrays as reported in Rodríguez et al (1998a, 2000). At each SAO iteration, a set of design points is selected for sampling using a DOE array. The design points are evaluated using the local disciplinary design tools, where linear approximations are used for the non-local input states. The resulting database is used to build a RSA. Many other research studies have combined DOE techniques and RSA for optimization.<sup>1;4;6;7;20</sup>

Rodríguez et al (2000) performed a comparison between the optimization based data generation (RS-CSSO) and a statistical based DOE approach using orthogonal arrays (OA). Results of that study show that while low strength orthogonal arrays seem to perform

well compared to the RS-CSSO approach, RS-CSSO is still more robust in driving the optimization. An attempt to overcome the natural advantages of the optimization based sampling was investigated in Pérez et al.(2000). In the Pérez study the DOE based sampling strategy was modified by projecting the orthogonal arrays onto the linearized descent feasible region. The results indicate that there is evidence that the RSA constructed with such a database, provides a better approximation of the system when constrained optimization is performed.

## 2 Design of Experiments

Several techniques have been developed to efficiently sample the design space and generate a proper response surface approximations. Among the common techniques to generate an experimental design are the traditional DOE arrays such as the full factorial experiments (FF), central composite design (CCD), Latin hypercubes and their extensions, the orthogonal arrays (OA's)(Owen, 1992; Hedayat et al.1999). Some quality improvement computer experiments such as D-optimality are too large or too complex for a SAO framework. OAs are an excellent choice for computer experiments because they are easy to generate. Owen (1992) has compiled a suite of programs to generate a broad class of OA's for different number of levels and design variables. They are space filling, covering the sampling region uniformly in the  $t$ -dimensional projection, where  $t$  is the strength of the OA. And finally the number design points is relatively small. In the construction of RSAs for MDO one important consideration is the dimensionality of the problem, where large problems may impose the *curse of dimensionality*. While small problems can be dealt easily with traditional sampling techniques (FF, CCD), as the number of variables increases, the complexity of the sampling does too. In the case of a second order RSA, the number of the parameters to be fitted is of the order  $O(n^2)$ . FF and CCD generate design arrays with order  $O(2^n)$  while some OA's have order  $O(n^2)$  without losing the space filling property.

## 3 Adaptive Experimental Design

The most important difference, from an experimental point of view, between traditional laboratory experiments and the computational experiments embedded in SAO, is that in the latter the experiment is repeated several times at different locations, up to convergence or stopping of the algorithm. At each new iteration a new sampling is performed of the same system but in a new sampling re-

gion. However we are not completely blind about the behavior of the system, as we have the previous information about the nature of the response surface, and the fitted coefficients of the previous local approximation. Due to the highly nonlinear nature of MDO problems, we do not expect to have the same response from the starting sampling region to the final one, and therefore the performance of a fixed experimental array may vary through the process. This fact was acknowledged in the research of Rodríguez *et al.* (2000) where the OA's were randomized to avoid having a fixed experimental array not capturing the true interactions of the design variables.

An adaptive experimental design that takes advantage of the information from the previous local approximation to modify the experimental array for the next sampling appears to hold promise for improving the efficiency of SAO algorithms. In this paper we investigate the use of information already available from the previous approximation to reduce the size of the experimental design while maintaining the quality of the approximation. As a result, we reduce the total cost of the optimization.

The number of parameters needed to fit a full second order approximation is  $O(n^2)$ . We can decrease this number to order  $O(n)$  by neglecting the off-diagonal terms. However these terms could be an important component of the second order information and thus we would end up by having a poor representation of the system response. What we propose in this paper is to transform the matrix of second order terms into its canonical form, that is, transforming the design space so that the off-diagonal components of the second order matrix (i.e., Hessian) can be temporarily neglected. Once we have found the transformation matrix we can assume, at least for some fixed number of iterations, that the curvature of the function will be invariant, so we compute only the main diagonal terms, which are  $O(n)$ .

#### 4 Trust Region Augmented Lagrangian SAO framework

In this paper the adaptive experimental design methodology has been implemented within the Trust Region Augmented Lagrangian algorithm of Rodríguez *et al.* (1998b). The implementation is tested using a suite of MDO test problems and the results compared with those using a fixed experimental design.

In the Sequential Approximate Optimization strategies of Wujek and Renaud<sup>27;28</sup> and Rodríguez *et al.*<sup>(16;17)</sup> which were modified for DOE based sampling in Rodríguez *et al.*<sup>18</sup> and Perez *et al.*<sup>12;13</sup> the framework constructs second order response surface approximations

of the objective function and constraints within a local trust region. The approximations are constructed using exact first order information available at the end of each SAO iteration, therefore the work of constructing a response surface involves only the fitting of the Hessian matrix  $H$ . Instead of using high fidelity data from the costly system analysis, variable fidelity can be collected using an optimization based sampling as in<sup>15;16;27;28</sup> or DOE<sup>17;18;12;13</sup>.

#### 5 Proposed methodology

The number of parameters to be estimated for a quadratic approximation assuming first order information is known, is  $\frac{n(n+1)}{2}$ . In this study we want to reduce the number of terms required for the approximation. One approach would be to arbitrarily set the off-diagonal terms to zero and fit only the main diagonal terms. While this certainly reduces the order of data to be queried to  $O(n)$ , the quality of the approximation might decrease considerably. An alternate approach can be taken. Once the full matrix of second order terms is approximated for a given design point, it can be transformed to its canonical form, i. e.. it can be diagonalized. In the process, we find a transformation matrix which rotates the space and aligns it so that the off-diagonal terms of the second order matrix vanish. In the next iteration, in the transformed design space, only the main diagonal of the second order matrix is fitted. As a result, back in the normal space a full matrix is obtained. Note that the transformation matrix can be kept as long as the curvature of the function does not change too much. In that case, the full matrix of second order terms has to be updated and a new transformation matrix can be computed.

The matrix of second order terms is symmetric. A diagonal decomposition of a symmetric matrix can be accomplished using eigenvalue decomposition. Since the eigenvectors are orthogonal to each other, the eigenvector matrix can be used to transform the design space for the next series of iterations. The eigenvalue problem can be posed as:

$$\mathbf{H}\mathbf{U} = \mathbf{U}\mathbf{H}_U, \quad (1)$$

where  $\mathbf{H}$  is the Hessian matrix,  $\mathbf{U}$  is the eigenvector matrix and  $\mathbf{H}_U$  is the diagonal eigenvalue matrix. The eigenvectors for a symmetric matrix are orthonormal, so the transformed space is just rotated with respect to the original one. Moreover, as the eigenvector matrix is or-

thonormal, the inverse transformation is cheap to evaluate. The direct and inverse transformation are performed by:

$$\mathbf{H}_U = \mathbf{U}^T \mathbf{H} \mathbf{U}, \quad (2)$$

$$\mathbf{H} = \mathbf{U} \mathbf{H}_U \mathbf{U}^T \quad (3)$$

Note that we have to transform the data to perform the least squares fitting. From a Taylor series, the second order contribution can be written as

$$\frac{1}{2} \mathbf{x}^T \mathbf{H} \mathbf{x}. \quad (4)$$

Using (3) and omitting the constant term we have

$$\mathbf{x}^T \mathbf{U} \mathbf{H}_U \mathbf{U}^T \mathbf{x}. \quad (5)$$

We then can apply the direct and inverse transformations of  $x$  giving

$$\mathbf{x}_U = \mathbf{U}^T \mathbf{x} \quad (6)$$

$$\mathbf{x} = \mathbf{U} \mathbf{x}_U. \quad (7)$$

The gradient transformation is

$$\nabla_{x_U} = \mathbf{U}^T \nabla_x \quad (8)$$

$$\nabla_x = \mathbf{U} \nabla_{x_U}. \quad (9)$$

Having defined the transformation matrix  $\mathbf{U}$ . We can assume, at least for some fixed number of iterations, that the eigenvectors will be invariant, but not their eigenvalues. Therefore we need to just estimate  $n$  parameters instead of the  $\frac{n(n+1)}{2}$  previously required.

### 5.1 An alternate approach.

In MDO, it is common to have several constraints in the formulation of a problem. The objective function and the constraints are often functions of the outputs

of coupled simulation codes, and thus RSAs are used to approximate them. A direct application of the methodology described above in a problem with  $m$  constraints, implies that  $m + 1$  least squares estimations would have to be done. For each function, an eigenvalue decomposition of its Hessian matrix, an individual database transformation and a least squares estimation have to be performed. We refer to this as the Individual Transformation (IT) method.

In a SAO framework, the optimization is performed over the unconstrained augmented Lagrangian, with variable bounds. Therefore the most important issue is to make a good fit of the augmented Lagrangian. We can find the transformation matrix for the augmented Lagrangian and use it as a single transformation to fit all the function and constraints. To this aim we have to derive the Hessian of the augmented Lagrangian.

In the SAO framework employed in this research each of the objective function and constraints are approximated by second order Taylor series approximation. Let's define the approximate objective function and constraints as:

$$\tilde{f} = f_0 + \nabla f_0^T + \frac{1}{2} \Delta \mathbf{x}' \mathbf{H}_{f_0} \Delta \mathbf{x} \quad (10)$$

$$\tilde{g}_i = g_{i0} + \nabla g_{i0}^T + \frac{1}{2} \Delta \mathbf{x}' \mathbf{H}_{g_{i0}} \Delta \mathbf{x}. \quad (11)$$

Without losing generality, and in order to simplify the derivation, we will include only inequality constraints in this paper, however the extension to include equality constraints is straightforward. The approximate augmented Lagrangian is:

$$\tilde{\Phi} = \tilde{f} + \lambda^T \tilde{\Psi} + r_p \tilde{\Psi}^T \tilde{\Psi} \quad (12)$$

$$\tilde{\Psi}_i = \min(\tilde{g}_i, -2 \frac{\lambda_i}{r_p}) \quad (13)$$

And we can write it in terms of the Taylor series approximation as:

$$\begin{aligned} \tilde{\Phi} = & \Phi_0 + \nabla \Phi_0^T \Delta \mathbf{x} + \frac{1}{2} \Delta \mathbf{x}' \mathbf{H}_{\Phi_0} \Delta \mathbf{x} + \\ & + O(\Delta \mathbf{x}^3) + O(\Delta \mathbf{x}^4) \end{aligned} \quad (14)$$

where we are interested in the matrix of second order terms  $\mathbf{H}_{\Phi_0}$ . Throughout the remainder of this paper we

will refer to this matrix of second order terms as the Hessian. *Keep in mind that Hessian terms are evaluated using response surface techniques that fits the second order response over the entire trust region.* Substituting 10 and 11 into 12 and associating terms we obtain:

$$\mathbf{H}_{\Phi_0} = \mathbf{H}_{f_0} + \sum_i \lambda_i \mathbf{H}_{\Psi_{i0}} + 2r_p \sum_i (\nabla \Psi_{i0} \nabla \Psi_{i0}^T + \Psi_{i0} \mathbf{H}_{\Psi_{i0}}) \quad (15)$$

Note that the expression for  $\mathbf{H}_{\Phi_0}$  contains both first and second order terms. First order information is already available, so we can combine the first and second order terms into single terms:

$$\mathbf{H}_{\Phi_0} = \mathbf{H}_{\Phi^{so}_0} + \mathbf{H}_{\Phi^{fo}_0}, \quad (16)$$

where

$$\mathbf{H}_{\Phi^{fo}_0} = 2r_p \sum_i \nabla \Psi_{i0} \nabla \Psi_{i0}^T \quad (17)$$

$$\mathbf{H}_{\Phi^{so}_0} = \mathbf{H}_{f_0} + \sum_i \lambda_i \mathbf{H}_{g_{i0}} + 2r_p \sum_i \Psi_{i0} \mathbf{H}_{\Psi_{i0}} \quad (18)$$

$\mathbf{H}_{\Phi^{fo}_0}$  is known. The matrix  $\mathbf{H}_{\Phi^{so}_0}$  is a linear combination of the objective function and constraint Hessians. If we find a transformation matrix such that in that transformed space the off-diagonal terms of  $\mathbf{H}_{\Phi^{so}_0}$  are negligible, there is no need to compute the individual off-diagonal terms of the objective function and constraints, as they will cancel with each other. Therefore we can use the eigenvector matrix of  $\mathbf{H}_{\Phi^{so}_0}$  to transform the design space and fit in that space the main diagonals of all the function. We call this the Cumulative Hessian (CH) approach.

It is important to note that though the function  $\Psi_i$  has been shown second order discontinuous, we can assume that for an active constraint  $g_i$ ,  $\mathbf{H}_{\Psi_{i0}} = \mathbf{H}_{g_{i0}}$  and for a non-active constraint  $\mathbf{H}_{\Psi_{i0}} = 0$ .

## 6 Implementation

A simple algorithm for the proposed methodology is given below. Additional implementation details can be found in the Test Problems section.

1. Query a database and compute the full Hessian matrix for each function involved ( $\mathbf{H}_i$ ).
2. Compute the transformation matrices (or matrix)  $\mathbf{U}_i$  ( $\mathbf{U}$ ):

Compute the eigenvector matrices  $\mathbf{U}_i$  of the Hessian for each function if the Individual Transformation is used, or

Compute the cumulative Hessian  $\mathbf{H}_{\Phi_0^{so}}$  as in (18) and compute its eigenvector matrix  $\mathbf{U}$ .

3. Optimize the approximate augmented Lagrangian with local variable bounds.
4. Query a reduced database to fit only  $n$  parameters.
5. In the transformed space(s)  $\mathcal{U}(\mathcal{U}_i)$ , compute the main diagonal terms of each Hessian.
6. Optimize the approximate augmented Lagrangian with local variable bounds.
7. If the approximation is satisfactory go to 4 if not, update the Hessians starting from 1

## 7 Test problems

To demonstrate the application of the decomposition technique within an SAO framework, we start with a simple two-dimensional problem.

### 7.1 Optimization of an unconstrained function.

To demonstrate how dramatic the results can be, we used a simple unconstrained problem in 2 dimensions:

$$\begin{aligned} \text{Minimize } f = & 3 + (x_1 - 40) + 2(x_2 - 40) + \\ & + 0.75(x_1 - 40)^2 + 0.75(x_2 - 40)^2 + \\ & + 0.5(x_1 - 40)(x_2 - 40) + 0.002x_1^2x_2 \quad (19) \end{aligned}$$

The optimum is located in  $x^* = (36.2564, 38.1618)$ . A simple SAO, with a fixed size of Trust Region radius, was performed using three methods to build the Hessian approximation: a full Hessian fit, the transformation method stated above and fitting just the main diagonal without transformation. In the first two cases, the optimum was located in 3 iterations, starting from a nearby point. However fitting just the main diagonal, the algorithm required 9 iterations to reach the optimum with a tolerance of  $dx \leq 0.01$ , and with a smaller tolerance ( $dx \leq 0.0001$ ) it required more that 300 iterations to converge as compared to 3 for the full Hessian or transformation method.

While actual engineering problems are more complex and restrictive than this unconstrained problem, it does

illustrate the potential of the proposed method. The additional examples given below represent more complex constrained problems that are closer to real engineering problems.

## 7.2 The Barnes problem

This is a purely mathematical two-dimensional problem and was originally formulated by G.K. Barnes as part of his Master's Thesis <sup>2</sup>. This problem was chosen because it is a 2 design variables problem which is highly nonlinear and therefore suitable for our needs. The problem is stated as:

$$\begin{aligned}
 \text{Minimize } f(\mathbf{x}, \mathbf{y}) &= a_1 + a_2x_1 + a_3y_4x_1 + a_5y_4^2 + \\
 &+ a_6x_2 + a_7y_1 + a_8x_1y_1 + a_9y_1y_4 + a_{10}y_2y_4 + \\
 &+ a_{11}y_3 + a_{12}x_2y_3 + a_{13}y_3^2 + \frac{a_{14}}{x_2 + 1} + a_{15}y_3y_4 + \\
 &+ a_{16}y_1y_4x_2 + a_{17}y_1y_3y_4 + a_{18}x_1y_3 + a_{19}y_1y_3 + \\
 &+ a_{20}e^{a_{21}y_1} \\
 \text{Subject to: } g_1 &= \frac{y}{700} - 1 \geq 0 \\
 g_2 &= \frac{x_2}{5} - \frac{y_4}{25^2} \geq 0 \\
 g_3 &= (y_5 - 1)^2 - \left(\frac{x_1}{500} - 0.11\right) \geq 0 \\
 0.0 \leq x_1 &\leq 75.0 \\
 0.0 \leq x_2 &\leq 65.0
 \end{aligned} \tag{20}$$

where the coefficients  $a$  are constants and their values can be found on Appendix A. The states are calculated by the CAs as:

$$\begin{aligned}
 CA_1 \quad y_1 &= x_1x_2 \\
 y_3 &= x_2^2 \\
 CA_2 \quad y_2 &= y_1x_1 \\
 y_4 &= x_1^2 \\
 y_5 &= \frac{x_2}{50}
 \end{aligned}$$

A plot of the design space is shown in Figure 1.

**7.2.1 Implementation details** Two iteration of SAO was performed starting from several design points. In the first iteration a full Hessian was fitted for each of the function and constraints. An optimization was performed using the approximate cumulative augmented Lagrangian with local variable bounds to find a new candidate point.

In the second iteration, a new database was generated around the current design point. With this database, the Hessian matrix was computed using the following methods:

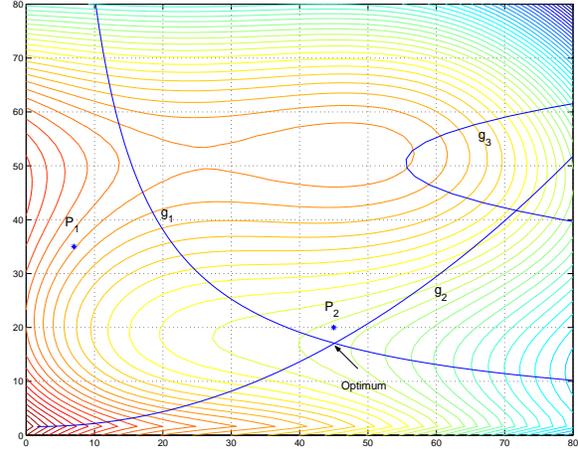


Figure 1. Design space of the Barnes problem

- Estimate the full Hessian matrix (FH).
- Estimate only the main diagonal terms of the Hessian without transformations (MD), in the original design space.
- Estimate the main diagonal in the transformed space:
  - One transformation matrix for each individual function involved (IT). The Hessian of each function is computed in its particular transformed space.
  - One transformation matrix from the cumulative Hessian (CH) of the Lagrangian. The eigenvector matrix of the cumulative Hessian as in (18) serves to transform the design space and the main diagonals of each Hessian are computed in this transformed design space.

Once the Hessian information was estimated, an optimization was performed on each of the four approximations computed. A new database was queried to calculate the mean square error of the augmented Lagrangian for each approximation.

The database was generated by sampling the Barnes function with a 9 point, 3 level, full factorial array. The database was queried within the limit of the local variable bounds defined as a fraction of the whole design space by the Trust Region radius  $\Delta$ .

**7.2.2 Results for the Barnes Problem** The results for two initial design points are given in this section. The first run started with point  $P_1 = (7, 35)$  which is an infeasible starting point that violates constraint 1. The sampling and optimization were performed in a trust re-

gion of  $\Delta = 0.1$ . Table 1 summarizes the results for each strategy used to fit the Hessian. In SAO the optimization is performed over the augmented Lagrangian, therefore we focus our results in the ability to capture the value of the Hessian matrix of the cumulative augmented Lagrangian as in Equation 18.

	$x_1^2$	$x_2^2$	$x_1x_2$	$x_1^*$	$x_2^*$	MSE
FH	0.1141	-0.0112	0.0254	11.125	31.425	1.2615e-3
MD	0.1141	-0.0112	0	11.125	31.425	1.4201e-2
IT	0.1145	-0.0118	0.0251	11.125	31.425	1.2631e-3
CH	0.1145	-0.0117	0.0251	11.125	31.425	1.3205e-3

Table 1. Point (7,35),  $\Delta = 0.1$

The first three columns denote the Hessian terms of the cumulative augmented Lagrangian:  $x_1^2, x_2^2, x_1x_2$ . We can see that while the Main Diagonal approach fits perfectly the  $x_1^2, x_2^2$  terms, the cross term is not captured although it has a somewhat negligible value. The Individual Transformation and the Cumulative Hessian strategies capture, with an acceptable accuracy, the main diagonal and off-diagonal terms. The small discrepancy in the results between the IT and the CH methods are due to the constraint violation, however the difference is not significant. The next two columns show the final result for the two step optimization:  $x_1^*, x_2^*$ . The final design is the same in all cases. Comparing the Mean Square Error (MSE) of the four RSAs we can see that the Main Diagonal approach generates a greater error (10 times greater) than those of the Individual Transformation and the Cumulative Hessian transformation. The magnitude of the last two is comparable to that of the Full Hessian fit.

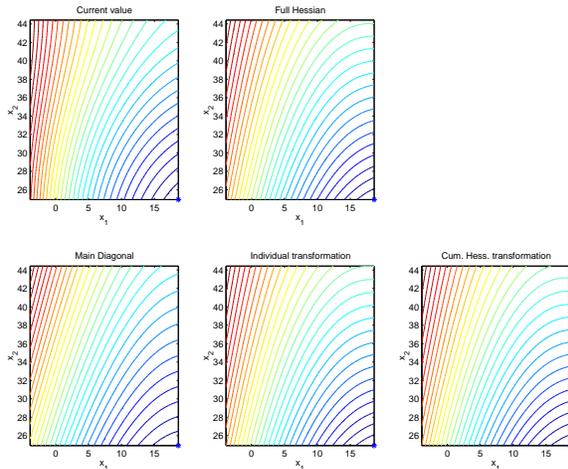


Figure 2. Augmented Lagrangian for point (7,35),  $\Delta = 0.3$

In the next run the size of the Trust Region radius was increased to  $\Delta = 0.3$  and the same starting point was used. Figure 2 shows the shape of the original Augmented Lagrangian and the four approximations. We can see that a slight change in shape is found in the Main Diagonal approach, however the minimum for the five plots is located in the lower right corner ( $x^* = (18.625, 24.925)$ ).

Results for the Hessian terms are found in Table 2. The maximum difference in Hessian terms is found in the off diagonal terms as the Main Diagonal approach does not compute them. The MSE shows a very small difference between the FH, IT and CH. The MSE for the MD approach is more than twice the value of the other three. However the four strategies end up at the same optimum.

	$x_1^2$	$x_2^2$	$x_1x_2$	$x_1^*$	$x_2^*$	MSE
FH	0.1143	-0.0095	0.0282	18.625	24.925	0.8933
MD	0.1143	-0.0095	0	18.625	24.925	2.0462
IT	0.1173	-0.0138	0.0261	18.625	24.925	0.8989
CH	0.1172	-0.0137	0.0261	18.625	24.925	0.9115

Table 2. Point (7,35),  $\Delta = 0.3$

The second point evaluated is  $x_0 = (45, 20)$ , which is located near the global optimum. A trust region of  $\Delta = 0.1$  is used in the same two iteration study. At this design point no constraint is violated but we are close to the feasible design boundaries of  $g_1$  and  $g_2$ . Results for this point are shown in Table 3. Results for IT and CH are the same as no constraint is being violated and therefore the augmented Lagrangian is reduced to the objective function \*. The MSE for the MD strategy is two orders of magnitude greater than the other three approaches, however the optimum with respect to the local variable bounds is found to be the same for each of the approximations.

	$x_1^2$	$x_2^2$	$x_1x_2$	$x_1^*$	$x_2^*$	MSE
FF	-0.0318	0.1549	0.0262	49.125	16.425	9.3201e-04
MD	-0.0318	0.1549	0	49.125	16.425	1.3077e-02
IT	-0.0316	0.1546	0.0264	49.125	16.425	9.3323e-04
CH	-0.0316	0.1546	0.0264	49.125	16.425	9.3323e-04

Table 3. Point (45,20),  $\Delta = 0.1$

\*We are performing a two step SAO. The Lagrangian multipliers are initialized to zero.

### 7.3 The Controls-Augmented Structure

This is an engineering design optimization problem called the Controls-Augmented Structure (CAS). This problem introduces more complexity with more design variables, more constraints and a fully coupled System Analysis (SA). One important feature of this problem is that the data used to construct the RSAs comes from the linearly decoupled subsystems (called Contributing Analysis or just CAs) instead of the costly SA.

The CAS design problem shown in Figure 3 was first introduced by Sobieszczanski-Sobieski *et al.*<sup>23</sup>. The problem consists of a total of 11 design variables and 43 states. The physical problem consists of a cantilever beam subjected to static loads along the beam and to a dynamic excitation force applied at the free end. Two sets of actuators are placed at the free end of the beam to control both the lateral and rotational displacement.

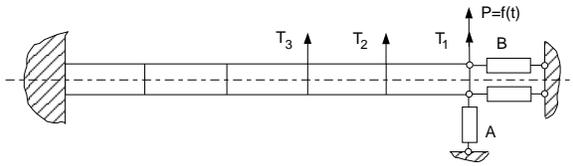


Figure 3. Controls-Augmented Structure.

The system analysis is comprised of two fully coupled contributing analysis (CAs) as shown in Figure 4. The structures subsystem, CA<sub>s</sub> consists of a finite element model of the beam where the natural frequencies and modes of the cantilever beam are computed. CA<sub>s</sub> requires, in addition to the characteristics of the beam, the weight of the control system as input. The weight of the control system is calculated in the controls CA, CA<sub>c</sub>. The weight of the control system is a function of the dynamic displacements and rotations of the free end of the beam. These dynamic displacements and rotations are functions of the natural frequencies and modes obtained in the structures CA, thus subjecting these CAs to coupling.

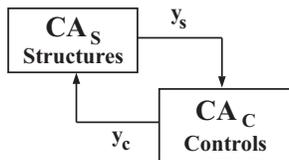


Figure 4. Dependency diagram of the CAS design problem.

The objective of the optimization is to minimize the total weight of the system  $W_t$ , composed of the weight of the beam  $W_s$  plus the weight of the control system  $W_c$ . The minimization is subject to seven constraints on the static stresses ( $\sigma$ ), static lateral and rotational displacements ( $dl$  and  $dr$ ), the first two natural frequencies ( $\omega_1$  and  $\omega_2$ ) and dynamic lateral and rotational displacements at the free end of the beam ( $ddl$  and  $ddr$ ). The problem is posed as:

$$\min W_t = W_s + W_c$$

subject to

$$g_1 = 1 - \frac{dl}{dl_a} \geq 0,$$

$$g_2 = 1 - \frac{dr}{dr_a} \geq 0,$$

$$g_3 = \frac{\omega_1}{\omega_{1a}} - 1 \geq 0,$$

$$g_4 = \frac{\omega_2}{\omega_{2a}} - 1 \geq 0,$$

$$g_5 = 1 - \frac{\sigma}{\sigma_a} \geq 0,$$

$$g_6 = 1 - \frac{ddl}{ddl_a} \geq 0,$$

$$g_7 = 1 - \frac{ddr}{ddr_a} \geq 0,$$

**7.3.1 Implementation details** In testing our methodology on this problem we perform a fully converged SAO constructing the Hessian of the objective functions and constraints using the strategies described in the previous sections. We use the Trust Region Augmented Lagrangian framework for SAO developed in Rodríguez *et al.*<sup>16:17</sup>. The response surface approximations were constructed with medium fidelity information queried by Orthogonal Arrays of strength 2 (see<sup>18</sup>) This means that the sampling is performed over the decoupled CA instead of sampling the costly System Analysis. At the beginning of the optimization the Full Hessians of the functions were computed. Transformation matrices were then computed for each of the decomposition strategies described above (i.e., IT and CH). When a negative Trust Region ratio was encountered, a full Hessian update was performed.

The problem has 11 design variables and therefore 66 Hessian terms. When a full Hessian update was required an OA with 128 points, 8 levels and strength 2 was

used. When only the 11 main diagonal components were computed (either in the transformed or non transformed space) smaller OAs are implemented. In total 4 OAs with an increasing number of design points were implemented : OA(27,13,3,2) 27 design points, 13 design variables (2 were cut), 3 levels, strength 2; OA(36,13,3,2) 36 design points, 13 design variables (2 were cut), 3 levels, strength 2; OA(50,11,5,2) 50 design points, 11 design variables, 5 levels strength 2 and the same OA(128,11,8,2) used for the full Hessian approximation. †

As described in <sup>11</sup> we can randomize an OA to have different experimental arrays. In this study, to avoid bias due to a particular experimental array from the randomization of the OAs, 10 runs were performed for each strategy and each OA. The results shown correspond to the average results of the 10 runs.

**7.3.2 Results for the CAS problem** The optimization was performed starting from two different points. The first is a feasible design ( $X_0 = (10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 0.1)$ ). The comparison of the four methodologies was done by evaluating the number of cycles required to converge (# of Approximate Minimizations) and the total number of CA calls required. The last one is the most important to evaluate the cost of the optimization, since each CA can be computationally expensive and thus the total number of CA calls is a measure of the computational cost.

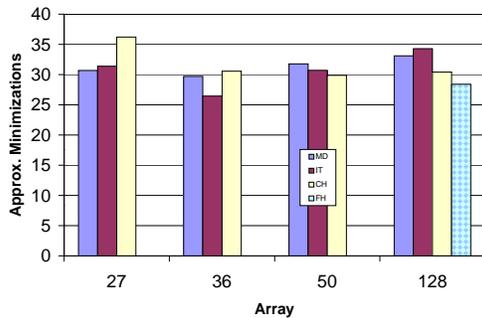


Figure 5. Starting from a feasible point. Approx. minimizations, CAS problem.

The number of Approx. optimizations is shown in Figure 5. There is no significant change in the number

† OA(27,13,3,2), OA(36,13,3,2), OA(50,11,5,2) can be found in <sup>8</sup>. OA(128,11,8,2) were generated using software by Owen <sup>11</sup>

of approximate minimizations required to converge the SAO. The CH strategy with the OA(27) required more than 35 iterations to converge. On the other hand using IT with OA(36) required the least number of approximate minimizations. We have to highlight that contrary to what we expected, for the MD and IT, the use of more design point increased the number of approximate minimizations. The results, in general illustrate that an order  $O(n)$  update for this problem works well without affecting the overall performance of the optimization. Figure

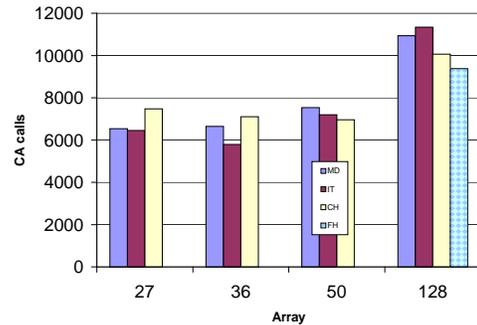


Figure 6. Starting from a feasible point. CA calls, CAS problem.

6 shows the results for the total cost of the optimization. We have to compare the cost of each run with the total cost of using a Full Hessian update. We can see an overall decrease of 35% in the total number of CA calls required to converge the SAO. It is important to remember that no special heuristic other than a negative TR ratio was used to decide when to perform a full Hessian update. Thus a further reduction could be possible with the proper algorithm.

The second starting design point is infeasible ( $P_2 = (5.0, 5.0, 5.0, 5.0, 5.0, 5.0, 5.0, 5.0, 5.0, 5.0, 0.1)$ ). Results are shown in Figures 7 and 8. In general, the number of approximate minimizations decreased for each strategy, as the number of design points in the OA increased. This result was expected as more design points provide more degrees of freedom in the least squares fit. For each OA, the MD strategy required more iterations than the IT, and the IT more than the CH except in the case of OA(128).

The savings in the number of CA calls is more dramatic for this starting point. The smallest number of CA are required when using the OA(27), however OA(36) and OA(50) do not significantly increase the number of CA calls required for SAO convergence. We can conclude that the second order off-diagonal terms are in-

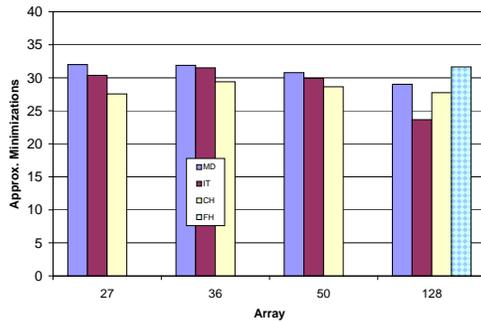


Figure 7. Starting from an infeasible point. Approx. minimizations, CAS problem.

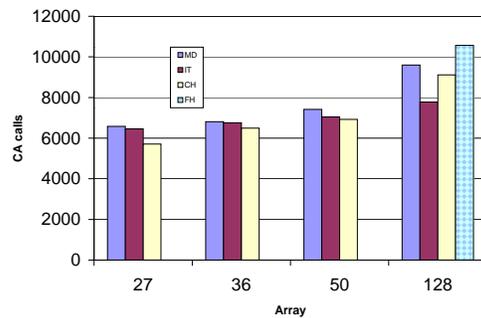


Figure 8. Starting from an infeasible point. CA calls, CAS problem.

significant, and that the augmented Lagrangian approximates well using just the main diagonal terms. Although small improvements are observed when using the proposed transformation techniques.

## 8 Discussion and concluding remarks

In this paper a methodology which reduces the size of the database required for building a quadratic response surface approximation is presented. The method makes use of a canonical transformation of the previous Hessian matrix used within a sequential approximate optimization. The method only requires computation of the main diagonal terms in the transformed space thereby reducing the amount of data required. Two variants of the method-

ology are presented. In one the Individual Transformation method, the transformation is applied individually to the objective function and each of the constraints. An alternate method which finds the Cumulative Hessian of the augmented Lagrangian and uses it to define the transformation is also presented. The methodology is applied in three test problems. The results are compared to those obtained by fitting the main diagonal only, without transformation and by fitting the whole Hessian matrix. Results show that the methodology can be applied to engineering problems, significantly reducing the amount of data required to fit a full quadratic function. Moreover the reduction is expected to increase as the number of design variables in the problem is increased, as the proposed model reduces the number of parameters to be fitted from  $O(n^2)$  to  $O(n)$ . While the multidisciplinary design optimization test problem did not show a noticeable difference between the proposed methodology and that of just fitting the main diagonal, the advantage was observed in the smaller example problems, where the use of the proposed method outperformed significantly the use of a main diagonal strategy. No significant difference has been observed between the two decomposition strategies IT and CH. Future research will focus on rotating the experimental array and aligning it to the transformation matrix, in order to reduce the cross coupling in the least squares problem.

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#### A Coefficients for the Barnes problem

$a_1$	75.196	$a_2$	-3.8112
$a_3$	0.12694	$a_4$	-2.0567e-3
$a_5$	1.0345e-5	$a_6$	-6.8306
$a_7$	0.030234	$a_8$	-1.28134e-3
$a_9$	3.5256e-5	$a_{10}$	-2.266e-7
$a_{11}$	0.25645	$a_{12}$	-3.4604e-3
$a_{13}$	1.3514e-5	$a_{14}$	-28.106
$a_{15}$	-5.2375e-6	$a_{16}$	-6.3e-8
$a_{17}$	7.0e-10	$a_{18}$	3.4054e-4
$a_{19}$	-1.6638e-6	$a_{20}$	-2.8673
$a_{21}$	0.0005		