Subproblem Optimization With Regression and Neural Network Approximators

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Abstract

Design optimization of large systems can be attempted through a subproblem strategy. In this strategy, the original problem is divided into a number of smaller problems that are clustered together to obtain a sequence of subproblems. Solution to the large problem is attempted iteratively through repeated solutions to the modest subproblems. This strategy is applicable to structures and to multidisciplinary systems. For structures, clustering the substructures generates the sequence of subproblems. For a multidisciplinary system, individual disciplines, accounting for coupling, can be considered as subproblems. A subproblem, if required, can be further broken down to accommodate subdisciplines. The subproblem strategy is being implemented into the NASA design optimization test bed, referred to as "CometBoards." Neural network and regression approximators are employed for reanalysis and sensitivity analysis calculations at the subproblem level. The strategy has been implemented in sequential as well as parallel computational environments. This strategy, which attempts to alleviate algorithmic and reanalysis deficiencies, has the potential to become a powerful design tool. However, several issues have to be addressed before its full potential can be harnessed. This paper illustrates the strategy and addresses some issues.

Introduction

Convergence difficulty can be encountered when nonlinear mathematical optimization methods are used to solve large multidisciplinary problems with many design variables and numerous behavior constraints. Solution to such problems can be attempted through a subproblem strategy in which the original problem is replaced by an equivalent sequence of subproblems as shown in figure 1. A subproblem with a few design variables and a small number of constraints can be solved with available nonlinear programming algorithms. Solution to the larger problem can be attempted by repeating solutions to the sequence of modest optimization subproblems until convergence is achieved for the original problem. This strategy is applicable to structures and to multidisciplinary systems. For structures, clustering substructures generates the sequence of subproblems. For a multidisciplinary system, individual disciplines, accounting for coupling, can be considered as subproblems. A subproblem, if required, can be further broken down to accommodate subdisciplines.

The subproblem strategy is being implemented into the NASA design optimization test bed, referred to as "CometBoards" (ref. 1). Neural network and regression approximators are employed for reanalysis and sensitivity analysis calculations at the subproblem level. The strategy is available in sequential as well as parallel computational environments. This strategy, which attempts to alleviate algorithmic and reanalysis deficiencies, has the potential to become a powerful design tool. However,
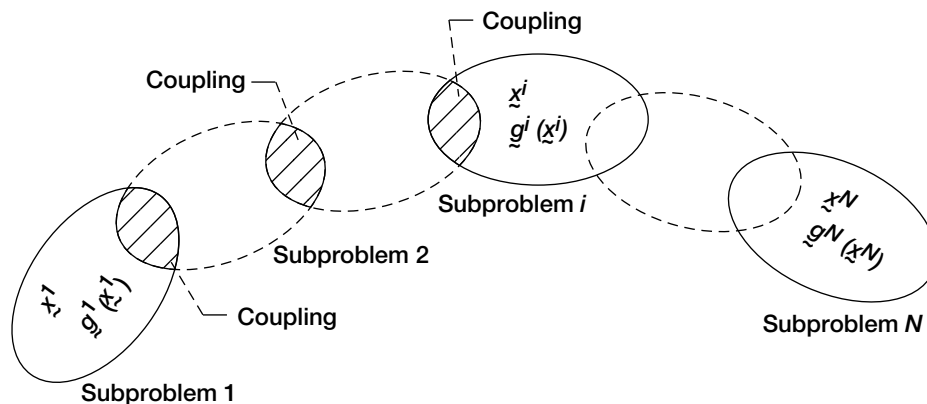
Figure 1.—Subproblem coupling.

several issues have to be addressed before its full potential can be harnessed. This paper addresses and illustrates issues relating to analysis approximations and convergence to local solutions. The paper is presented in these subsequent sections: design test bed CometBoards; subproblem solution strategy; analysis approximation; illustrative example; convergence to local solutions; and conclusions.

Design Test Bed CometBoards

The test bed CometBoards, an acronym meaning comparative evaluation test bed of optimization and analysis routines for the design of structures, was originally developed to compare different nonlinear mathematical programming algorithms and different analysis methods for structural design applications. The test bed was subsequently expanded for multidisciplinary design problems. Its modular organization is shown in figure 2. The CometBoards system first formulates the design as a nonlinear mathematical programming problem, reading information specified in input data files that include initial design with upper and lower bounds, limitation on behavior constraints, definition of subproblems, cascade strategy (ref. 2), and so forth. It then solves the resulting problem by executing the required segments of the program.

Problem formulation can use several types of analysis tools available in its analyzer module. The analyzers available include LE_HOST (ref. 3) and COSMIC/NASTRAN (ref. 4) for structural analysis, FLOPS (flight optimization system for aircraft analysis, ref. 5), NEPP (NASA Engine Performance Program for air-breathing engine cycle analysis, ref. 6), and others. Alternatively, a user-specified analyzer, which can be integrated through a soft coupling strategy, can be used. The solution to the optimization problem can use any one of a dozen optimization algorithms (ref. 7) available in CometBoards or can use a cascade strategy.

The cascade strategy is created by combining more than one optimizer in a specified sequence with pseudorandom perturbation between two optimizers. An approximation module with neural network and regression methods available in CometBoards can be used to reduce the number of calculations in optimization (refs. 8 and 9). The present version of CometBoards can accommodate several different disciplines, each of which can be further divided into subproblems. Thus, the CometBoards design tool can optimize a system that can be defined in terms of about 100 optimization subproblems. Alternatively, the CometBoards test bed can be used to examine the optimality of a small portion of a larger design problem by appropriate input data specification.
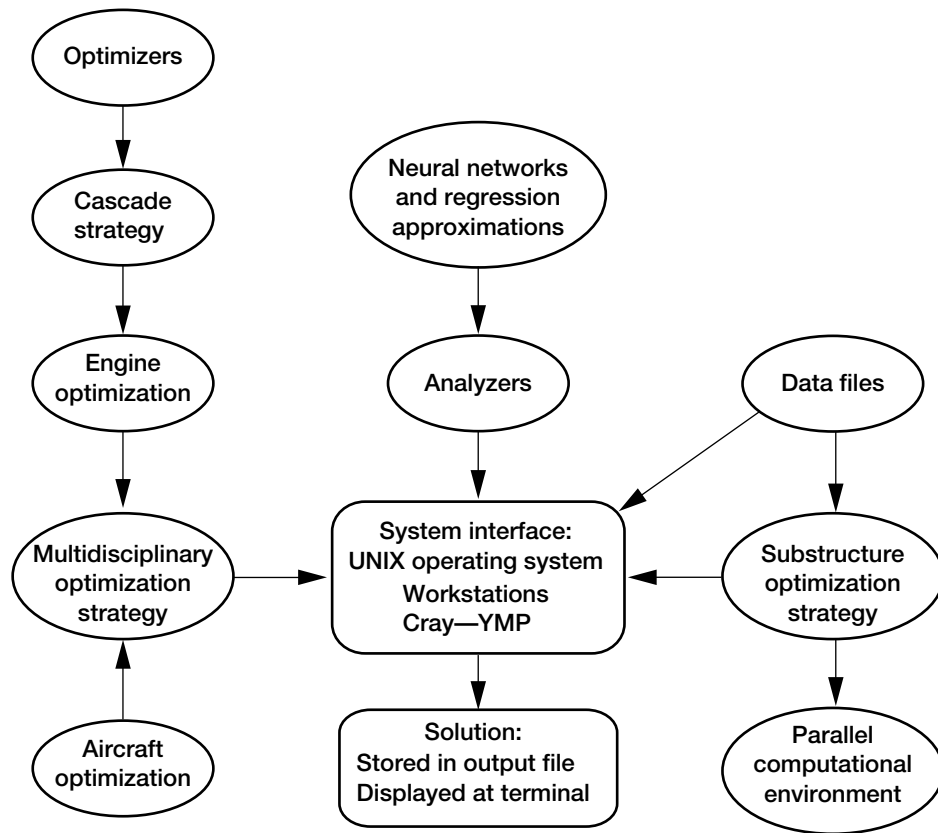
Figure 2.—Organization of CometBoards test bed.

Subproblem Solution Strategy

Subproblem solution strategies for sequential and parallel algorithms are depicted in the flow diagrams of figure 3. The flow diagrams each have two loops. The inner loop ($i = 1, N$) is associated with the optimization of N subproblems. In the parallel computational environment the subproblems are distributed to different processors. The outer loop repeats the solution of the N subproblems several times (referred to as "cycles") until convergence. In the sequential computational environment the subproblems are optimized in sequence, and the design variables for the entire structure (also referred to as "global variables") are updated as soon as a solution to any single subproblem is available. In parallel computation, wherein subproblems are assigned to different processors, the global design variables can be updated only after the solutions have been completed for all the subproblems. In other words, the sequential algorithm, which benefits from intermediate improvement to the global design variables, can converge faster than the parallel algorithm because updating the global variables in this scheme cannot proceed until a full subproblem optimization cycle has been completed.
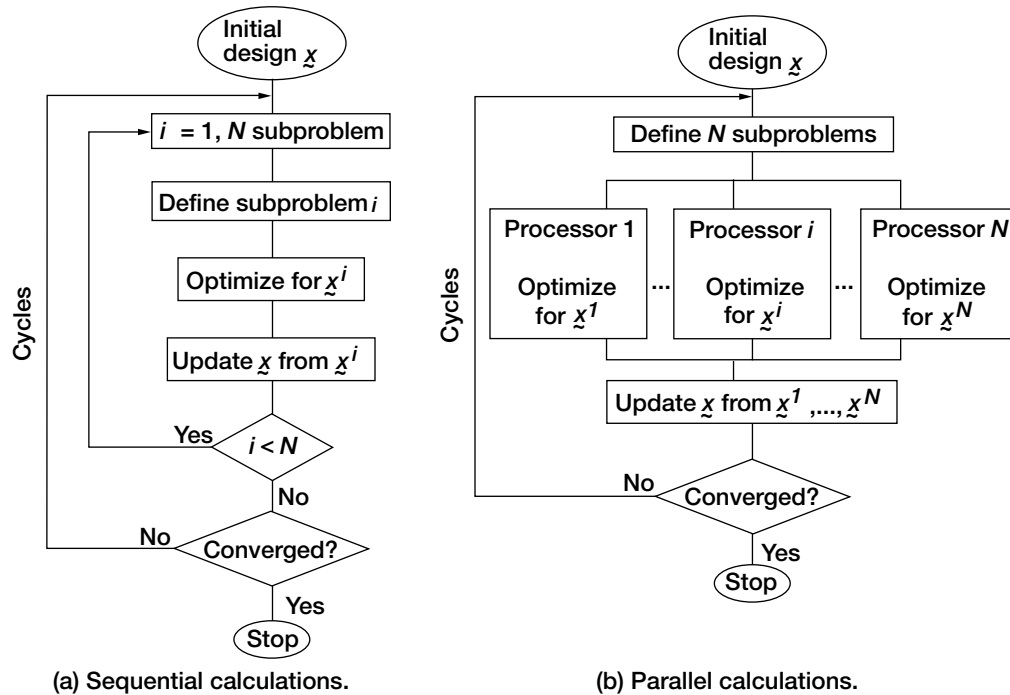
(a) Sequential calculations. (b) Parallel calculations.

Figure 3.—Substructure solution strategy.

Analysis Approximation

Approximation is employed to simplify analysis and reduce distortion of the design space. The salient features of analysis approximation are as follows:

1. Analysis approximation is carried out for each subproblem prior to its solution.

2. Objective function and the constraints are separately approximated. Provision exists to approximate a component of a constraint (such as the stress σ instead of the stress constraint $\{g = |\sigma/\sigma_0| - 1 \leq 0\}$). The approximation can be carried out either for the large number of raw constraints or after the constraint formulation.

3. The approximation provides the value of the function and its gradient with respect to the design variables.

4. Both the linear regression method and neural networks can be used for approximations. An approximate analyzer at a subproblem solution stage is formulated in the following steps:

(a) Select the basis functions.

(b) Establish a benchmark solution around which input-output pairs are chosen.

(c) Generate good-quality input-output pairs for objective function and constraints or their components.

(d) Train the approximate methods with validation. This process provides the constraints and their sensitivities.

(e) Use the approximators for the subproblem solution.

(f) Repeat steps (b–d) prior to each subproblem solution. Step (a) has to be performed once for the entire optimization process.

Linear Regression Analysis

The linear regression method available in CometBoards approximates a function by using the following basis functions: (1) a cubic polynomial, (2) a quadratic polynomial, (3) a linear polynomial in reciprocal variables, (4) a quadratic polynomial in reciprocal variables, and (5) combinations of these functions. The regression coefficients are determined by using the linear least-squares method in the LAPACK library (DGELS routine, ref. 10). The gradient matrix of the regression function with respect to the design variables is obtained in closed form. Once the regression coefficients have been obtained, the reanalysis and the sensitivity analyses require trivial computational effort.

Neural Network Approximations

The neural network approximation available in CometBoards is referred to as "Cometnet" (ref. 8). It approximates the function with a set of kernel functions. Cometnet permits approximations with linear and reciprocal polynomials, as well as with Cauchy and Gaussian radial functions. A singular-value decomposition algorithm is used to calculate the weight factors in the approximate function during network training. A clustering algorithm in conjunction with a competing complexity-based regularization algorithm is used to select suitable parameters for defining the radial functions.

Benchmark Solution and Input-Output Training Pairs

The initial design is considered as the benchmark solution for generating the input-output pairs for the first subproblem. For subsequent subproblems the benchmark solution is updated by using optimization solutions available at that iteration stage. For generating the input-output pairs to train the approximate methods, a set of design points is selected at random within their upper and lower bounds by using a design-of-experiment strategy. The number of input-output pairs and the bounds of the design variables are changed as the optimization iterations progress.

Training the Approximate Methods

Both the regression and neural network methods are trained for a set of good-quality input-output training pairs. The basis functions are made as identical as possible between the methods. Selection of similar basis functions allows a systematic comparison of the two approximation concepts. Consider, for example, substructure 1 of the trussed-ring problem subsequently described in this paper. The basis functions used in the regression method for this substructure consist of linear and quadratic polynomials in design variables and linear polynomials in reciprocal variables. For the substructure with eight design variables the basis function becomes a polynomial with 53 coefficients. Likewise, for the same substructure the neural network scheme has 53 coefficients. In other words, the number of coefficients in the numerical approximations is the same for both the neural network and regression methods.
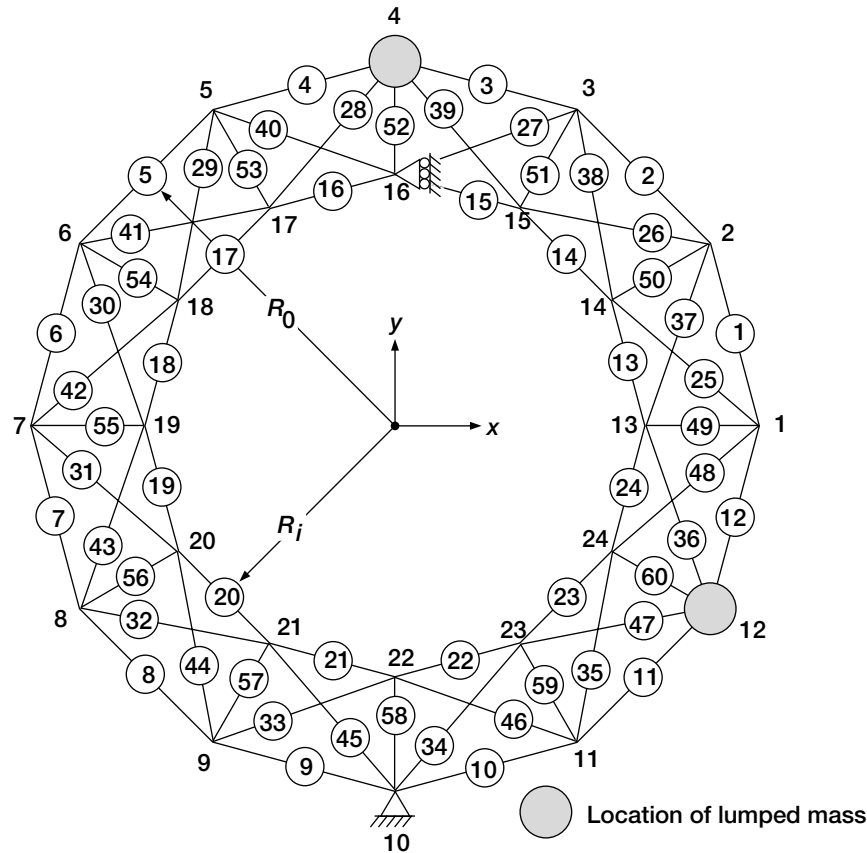
Figure 4.—Sixty-bar trussed ring.

Illustrative Example

The subproblem solution strategy is illustrated by considering the design of a modest trussed steel ring shown in figure 4, as an example. The ring is made of 60 bars with inner and outer diameters of 180 and 200 in., respectively. It is fully restrained at node 10 and free to move only along the y direction at the diametrically opposite node 16. The ring is subjected to two load conditions. The first load condition consists of a 40-kip compression along its horizontal diameter, applied at nodes 1 and 7. The second 40-kip load, applied at node 4, induces compression along the vertical diameter. For the purpose of design the 60 bar areas of the truss are linked to obtain 16 independent design variables. Sixty stress constraints (with a yield strength of 20 ksi), for each load condition, are grouped to obtain 16 constraints. The distortions of the ring along the horizontal and vertical diameters are controlled through 4-in. displacement limitations specified at nodes 1, 4, and 7 for each load condition. The ring is designed under problem 1 and problem 2. In problem 1 the optimum weight of the ring is obtained for stress and displacement constraints. Problem 2 includes all the constraints of problem 1 and a frequency limitation at 14 Hz. Subproblem solution is obtained in the following steps.

Step 1: Substructure Model

A substructure model for the ring is obtained by dividing it into four substructures. The substructures are described in table 1. Take, for example, substructure 1. It encompasses 12 bars that form the outer ring (see fig. 4). The 12 bar areas are linked to obtain four design variables. Likewise, the other three substructures are defined in table 1.

TABLE 1.—DESIGN VARIABLES AND SUBSTRUCTURES OF RING PROBLEM

Design variables	Area of bars	Substructures	Remarks
1	1,2,3	I	Outer ring northeast (see fig. 4)
2	4,5,6	I	Outer ring northwest
3	7,8,9	I	Outer ring southwest
4	10,11,12	I	Outer ring southeast
5	13,14,15	II	Inner ring northeast
6	16,17,18	II	Inner ring northwest
7	19,20,21	II	Inner ring southwest
8	22,23,24	II	Inner ring southeast
9	25,26,27,37,38,39	III	Crossbars northeast
10	28,29,30,40,41,42	III	Crossbars northwest
11	31,31,33,43,44,45	III	Crossbars southwest
12	34,35,36,46,47,48	III	Crossbars southeast
13	49,50,51	IV	Radial bars east and northeast
14	52,53,54	IV	Radial bars north and northwest
15	55,56,57	IV	Radial bars west and southwest
16	58,59,60	IV	Radial bars south and southeast

Step 2: Definition of Subproblems

The four substructures are clustered together to obtain four subproblems, as defined in table 2. For example, subproblem 1 is obtained by combining substructures III and I. It has eight design variables and eight stress and six displacement constraints for problem 1. One frequency constraint is added to obtain problem 2. Other subproblems are defined in table 2.

TABLE 2.—DEFINITION OF SUBPROBLEMS FOR RING PROBLEM

Subproblems	Substructures	Remarks
1	I and III	Outer ring and crossbars: 8 design variables; 8 stress and 6 displacement (and 1 frequency) constraints
2	II and IV	Inner ring and radial bars: 8 design variables; 8 stress and 6 displacement (and 1 frequency) constraints
3	II and III	Inner ring and crossbars: 8 design variables; 8 stress and 6 displacement (and 1 frequency) constraints
4	I and IV	Outer ring and radial bars: 8 design variables; 8 stress and 6 displacement (and 1 frequency) constraints

Step 3: Solution of Subproblems

The four subproblems are solved in a sequence, one after the other. Solution to the first subproblem is initiated from the specified initial design. For solution of subsequent problems the initial design is updated by using available subproblem solutions at that solution stage. Approximate analysis and sensitivity analysis models with neural network and regression methods are developed at the beginning of each subproblem design. Solution of all four subproblems represents one cycle. The cycling is repeated until satisfactory solution is obtained for the large problem.

Results for Ring Problem

Solution to each ring problem has been obtained for nine different cases. Summaries of results for the two problems are depicted in tables 3 and 4. The mean and the standard deviation are given for the design variables instead of their individual values. The nine test cases considered are described here.

Case 1.—The ring is designed as a single problem without the use of subproblem strategy or the approximation concepts. COSMIC/NASTRAN is the analysis tool. A sequential quadratic programming (SQP) algorithm is the optimizer. This design is considered the benchmark solution and all other results are compared with it. This solution was verified through a three-optimizer cascade strategy (method of feasible directions (FD), followed by SQP and the same FD). The cascade results confirmed the benchmark solution. The method of feasible directions produced a 0.5 percent error in the weight and a 0.9 percent mean-square error for the design variables. Mild infeasibility was noticed for a few constraints.

TABLE 3.—SOLUTIONS FOR RING PROBLEM WITH STRESS AND DISPLACEMENT CONSTRAINTS
(PROBLEM 1)

Test case	Description	Optimum weight, lb	Design variables, sq. in.		Number of active constraints	Number of cycles (number of subproblems)	CPU time to solution, min
			Mean	Standard deviation			
1	Single problem; COSMIC/NASTRAN analyzer; SQP optimizer (benchmark solution)	799.9	3.15	0.81	4 stress, 1 disp.	1 (1)	42.0
2	Four mutually exclusive subproblems; COSMIC/NASTRAN and SQP	1487.8	4.64	3.4		Failed	
3	Four coupled subproblems; COSMIC/NASTRAN and SQP	799.9	3.15	0.81	4 stress, 1 disp.	4 (16)	81.9
4	Four coupled subproblems; regression analyzer and SQP; constraint formulation active both at training and design stages	800.1	3.15	0.81	3 stress, 1 disp. (a)	3 (13)	------
5	Four coupled subproblems; regression analyzer and SQP; constraint formulation passive at both training and design stages	800.1	3.16	0.82	4 stress, 1 disp.	3 (13)	169.4
6	Four coupled subproblems; regression analyzer and SQP; constraint formulation passive at training but active at design stage	800.1	3.16	0.82	4 stress, 1 disp.	3 (13)	170.5
7	Same as case 4, using neural network analyzer	800.1	3.15	0.81	4 stress, 1 disp.	3 (13)	------
8	Same as case 5, using neural network analyzer	800.6	3.16	0.81	4 stress, 1 disp	3 (12)	------
9	Same as case 6, using neural network analyzer	800.1	3.16	0.82	4 stress, 1 disp.	3 (13)	197.6

[a]Infeasibility at a small fraction of 1 percent.

TABLE 4.—SOLUTIONS FOR RING PROBLEM WITH STRESS, DISPLACEMENT, AND FREQUENCY CONSTRAINTS
(PROBLEM 2)

Test case	Description	Optimum weight, lb	Design variables, sq. in.		Number of active constraints	Number of cycles (number of subproblems)	CPU time to solution, min
			Mean	Standard deviation			
1	Single problem; COSMIC/NASTRAN analyzer; SQP optimizer (benchmark solution)	900.0	3.52	1.08	8 stress, 1 frequency	1 (1)	80.5
2	Four mutually exclusive subproblems; COSMIC/NASTRAN and SQP	905.9	3.54	1.29	5 stress, 1 frequency	2 (8)	347.6
3	Four coupled subproblems; COSMIC/NASTRAN and SQP	899.9	3.50	1.09	7 stress, 1 frequency (a)	17 (68)	203.2
4	Four coupled subproblems; regression analyzer and SQP; constraint formulation active both at training and design stages	859.8	Infeasible at 55 percent and underdesign; failed				
5	Four coupled subproblems; regression analyzer and SQP; constraint formulation passive at both training and design stages	900.8	3.51	1.07	8 stress, 1 frequency (a)	3 (13)	288.9
6	Four coupled subproblems; regression analyzer and SQP; constraint formulation passive at training but active at design stage	900.8	3.51	1.07	8 stress, 1 frequency (a)	3 (13)	289.6
7	Same as case 4, using neural network analyzer	859.8	Failed				
8	Same as case 5, using neural network analyzer	900.6	3.51	1.07	8 stress, 1 frequency (a)	3 (13)	319.5
9	Same as case 6, using neural network analyzer	900.8	3.51	1.07	8 stress, 1 frequency (a)	3 (13)	320.9

[a]Infeasibility at a small fraction of 1 percent.

Case 2.—The ring problem is solved by using the subproblem strategy and neglecting substructure coupling. The COSMIC/NASTRAN and SQP algorithms were used as the analysis and design tools, respectively.

Case 3.—This case is identical to case 2, but substructure coupling is included.

Case 4.—The ring problem is solved by using four coupled subproblems. Analysis is approximated by a linear regression method, and the SQP algorithm is used. Sixteen grouped stress constraints, the displacement constraints, and the weight are approximated.

Case 5.—Case 5 is the same as case 4, but approximation is carried out for all 120 stress constraints. All 120 stress constraints are used during design optimization.

Case 6.—Case 6 is the same as case 5, but the 16 grouped stress constraints are used during design optimization.

Case 7.—Case 7 is the same as case 4, but linear regression is replaced by neural network approximation.

Case 8.—Case 8 is the same as case 5, but neural network approximation replaces the linear regression method.

Case 9.—Case 9 is the same as case 6, but linear regression is replaced by neural network approximation.

From the nine solution cases of problem 1 (see table 3) we observe the following:

1. The benchmark solution has an optimum weight of 800 lb. There are a total of five active constraints: four stress and one displacement. The mean value of the 16 design variables is 3.15 square in. with a standard deviation of 0.81 square in.

2. Out of the nine cases only case 2 (which excluded coupling between the substructures) failed to converge to the benchmark solution. The other eight cases produced acceptable solutions with minor variations.

3. Typically, a subproblem strategy required three design cycles corresponding to 13 subproblem solutions. Subproblem solution strategy is numerically more expensive than regular optimization. With the COSMIC/NASTRAN analyzer the subproblem strategy is twice as expensive as the regular optimization. The regression and neural network approximators increase the burden by four and five times, respectively. The generation of the approximate models consumes the bulk of calculations.

   Likewise from the nine solution cases of problem 2 (which included a frequency constraint; see table 4) we observe the following:

4. This benchmark solution has an optimum weight of 900 lb. There are a total of nine active constraints: eight stress and one frequency. No displacement constraint is active. The mean value of the 16 design variables is 3.52 square in. with a standard deviation of 1.08 square in.

5. Case 4 and case 7 failed to converge. Both cases trained a reduced number of stress constraints. Case 2, which failed earlier, was successful when a frequency constraint was included. Some variation is noticed in the number of active constraints for the nine cases.

6. The inclusion of a frequency constraint increased the computational burden by a factor of 2 with regular analyzers and by a factor of 1.5 with the approximators. Regular optimization with and without the frequency constraint required 80.5 and 42.0 CPU minutes, respectively. Likewise, the inclusion of the frequency (see case 5) increased solution time from 170 to 289 CPU minutes for the regression model. The neural network method for the same case 5 was 10 percent more expensive than the regression method. A typical subproblem strategy required three design cycles that correspond to 13 subproblem solutions.

Convergence to Local Solutions

The subproblem strategy had a tendency to converge to local solutions different from that obtained when regular optimization is used. It was also observed that the variation in the minimum weight between the solutions was small, less than 1 percent. This mild variation in weight is within the numerical accuracy of the algorithms. In other words, the minimum weight remained the same for the subproblem and regular optimization strategies. However, there was substantial variation in the design variables.

The optimum depth profiles for a beam obtained for different combinations of behavior constraints and two solution methods are depicted in figure 5. The depth of the beam varied by about 10 to 15 percent between the two solution methods. The beam profile is more uniform for regular optimization than for subproblem optimization. Subproblem and regular solutions produced the same weight and the same set of active constraints.
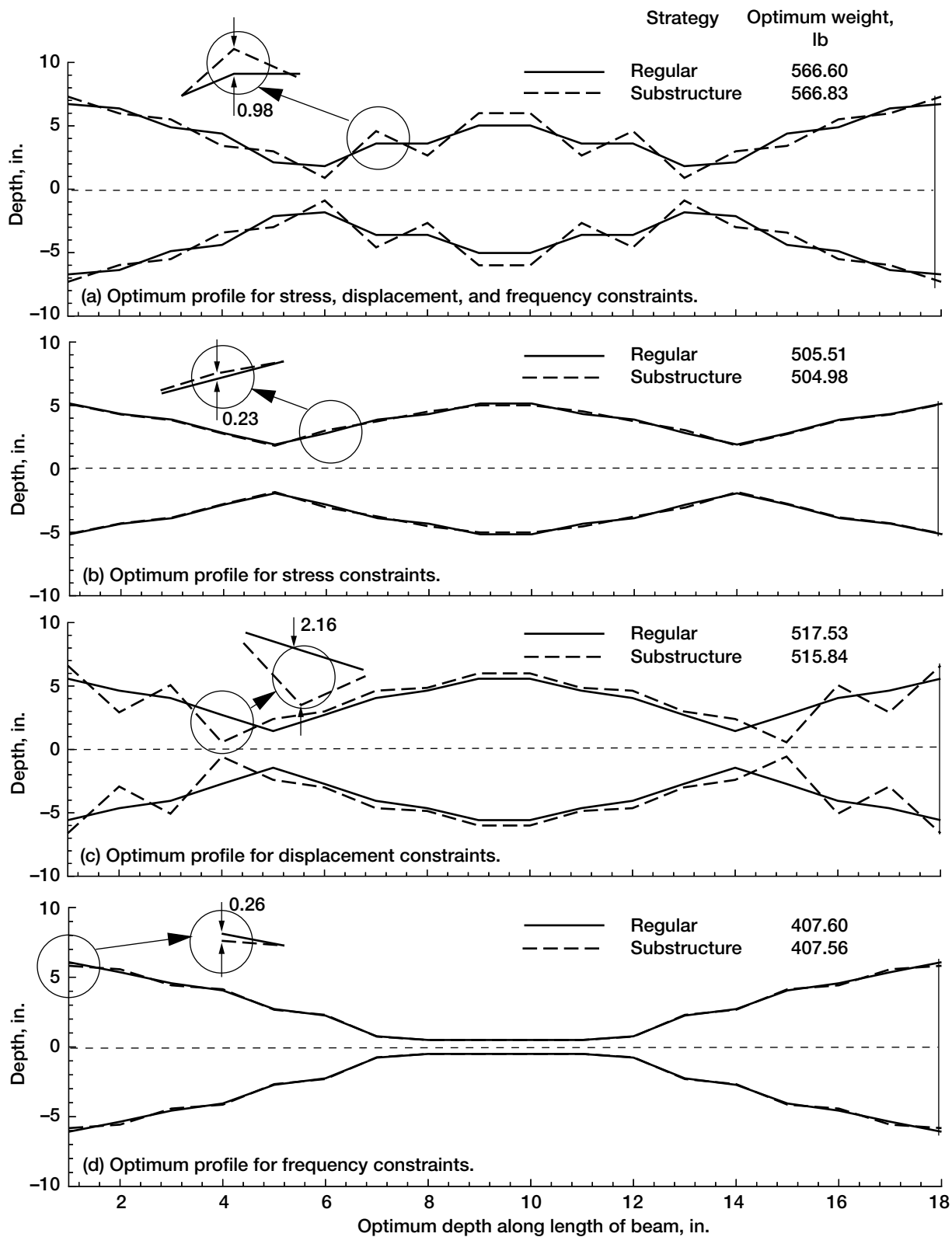
Figure 5.—Different optimum depth profiles for beam obtained with regular and substructure strategies.
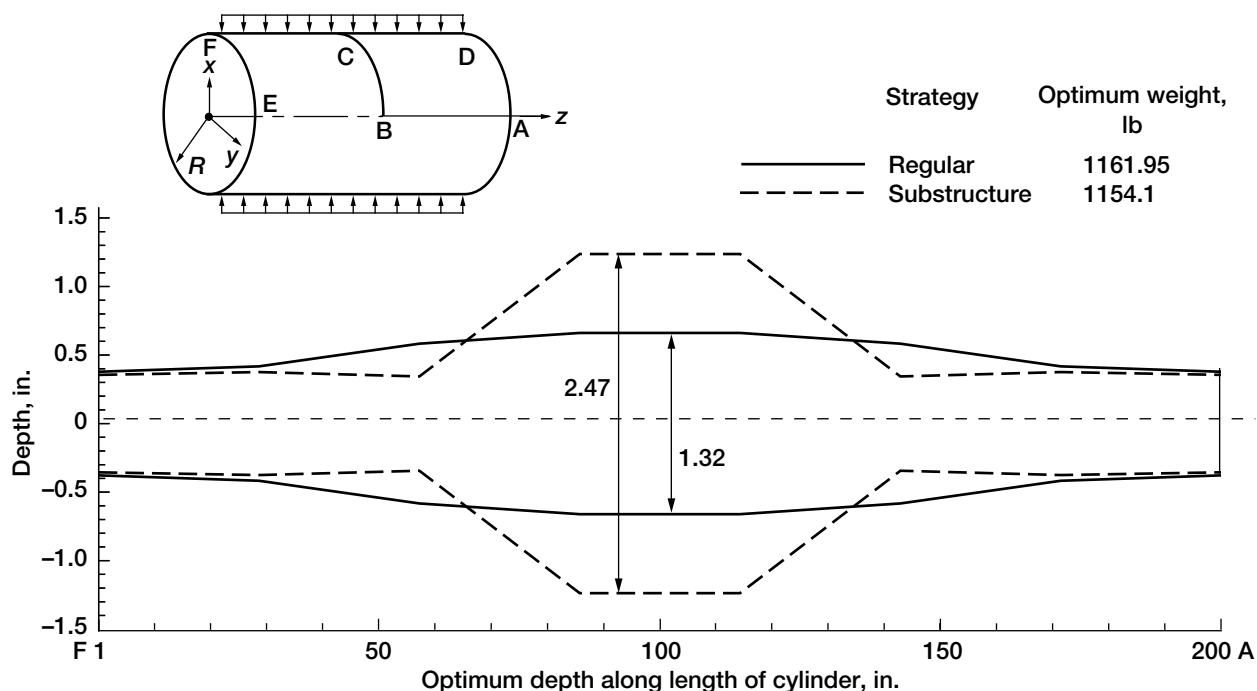
Figure 6.—Optimum depth profile for cylindrical shell with regular and substructure strategies for stress and displacement constraints.

The optimum depth profiles for a cylindrical shell obtained by using regular and subproblem strategies are depicted in figure 6. The profile generated from regular optimization is more uniform than that generated from substructure optimization. The optimum weights were 1161.95 and 1154.1 lb for the regular and substructure strategies, respectively. The difference of 0.676 percent can be considered negligible because of the complexity of the problem. The depth differed substantially between the two solutions. At the crown the optimum depths of 1.322 and 2.471 in. varied by 53 percent. At optimum the regular optimization and substructure strategies produced a different number of active constraints.

Conclusions

This study of subproblem solution strategy has led to the following conclusions:

1. Subproblem solution strategy has the potential to solve large problems. However, an adequate amount of coupling is required for a successful subproblem solution.

2. The subproblem strategy can be numerically more expensive than regular optimization.

3. Both neural network and regression methods provide adequate analysis models and perform at about the same level of efficiency.

4. Subproblem solution may produce an irregular design in contrast to regular optimization. Alleviation of this deficiency is important to the success of the strategy.

5. The training of the raw constraints instead of the formulated constraints requires additional research.

6. A larger size and fewer subproblems can improve the efficiency of the strategy.

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13. ABSTRACT (*Maximum 200 words*)

Design optimization of large systems can be attempted through a subproblem strategy. In this strategy, the original problem is divided into a number of smaller problems that are clustered together to obtain a sequence of subproblems. Solution to the large problem is attempted iteratively through repeated solutions to the modest subproblems. This strategy is applicable to structures and to multidisciplinary systems. For structures, clustering the substructures generates the sequence of subproblems. For a multidisciplinary system, individual disciplines, accounting for coupling, can be considered as subproblems. A subproblem, if required, can be further broken down to accommodate subdisciplines. The subproblem strategy is being implemented into the NASA design optimization test bed, referred to as "CometBoards." Neural network and regression approximators are employed for reanalysis and sensitivity analysis calculations at the subproblem level. The strategy has been implemented in sequential as well as parallel computational environments. This strategy, which attempts to alleviate algorithmic and reanalysis deficiencies, has the potential to become a powerful design tool. However, several issues have to be addressed before its full potential can be harnessed. This paper illustrates the strategy and addresses some issues.

14. SUBJECT TERMS

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