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# TRACING STRUCTURAL OPTIMA AS A FUNCTION OF AVAILABLE RESOURCES BY A HOMOTOPY METHOD\*

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Optimization problems are typically solved by starting with an initial estimate and proceeding iteratively to improve it until the optimum is found. The design points along the path from the initial estimate to the optimum are usually of no value. The present work proposes a strategy for tracing a path of optimum solutions parameterized by the amount of available resources. The paper specifically treats the optimum design of a structure to maximize its buckling load. Equations for the optimum path are obtained using Lagrange multipliers, and solved by a homotopy method. The solution path has several branches due to changes in the active constraint set and transitions from unimodal to bimodal solutions. The Lagrange multipliers and second-order optimality conditions are used to detect branching points and to switch to the optimum solution path. The procedure is applied to the design of a foundation which supports a column for maximum buckling load. Using the total available foundation stiffness as a homotopy parameter, a set of optimum foundation designs is obtained.

#### 1. Introduction

Optimization problems are typically solved by starting with an initial estimate and proceeding iteratively to improve it until the optimum is found. The design points along the path from the initial estimate to the optimum are usually of no value. However, this need not be the case. In many applications, it is of interest to find the family of optima obtained by varying an input parameter such as the amount of available resources. If one member of the family is known, it may be possible to use it as a starting point and to follow an optimization path that goes through the other members of the family.

A first step in tracing a family of optima is the application of sensitivity information to extrapolate from one member of the family to another. The present paper proposes the use of the sensitivity information to formulate the path of optima as the trajectory of a differential equation, a procedure known as a homotopy technique.

The basic theory of globally convergent (convergent from an arbitrary starting point) homotopy methods was developed in 1976 [1, 2]. Since then, the method has been used in a wide range of scientific and engineering problems. It has been successfully applied to nonlinear complementarity problems [3], nonlinear two-point boundary value problems [4], fluid dynamics problems [5, 6], and nonlinear elastica problems [7, 8]. References [9, 10] show

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the application to optimum structural design problems discretized by plane stress finite elements. Reference [9] shows that an appropriate homotopy method is globally convergent for an optimum design problem. For nonconvex problems the global convergence may be to only a local optimum design.

In this paper, the original globally convergent homotopy method is adapted to the design of an elastic foundation for maximizing the buckling load of a column. This problem has been solved before [11] for a limited range of resource (i.e., total foundation stiffness). The present paper shows how the solution process can start from the minimum amount of resources which is required for a feasible solution to the highest value that may be of interest.

#### 2. Optimization problem

The optimization problem that we consider here is to maximize the lowest buckling load of a structure for a given amount of resources. The structure is discretized by finite elements. Expressing the lowest buckling load with Rayleigh's quotient, the problem is written as

$$\max_{v} \min_{u} \frac{u^{t} K u}{u^{t} K_{G} u} , \tag{1}$$

such that  $c^{t}v - \theta = 0$  and

$$v_{i \min} \leq v_i \leq v_{i \max}$$
 for  $i = 1, \ldots, M$ ,

where v is a vector of design variables with components  $v_i$ , u is the displacement vector, K and  $K_G$  are the stiffness matrix and the geometric stiffness matrix, respectively, c is a positive cost vector, and  $\theta$  is the amount of available resources, representing total foundation stiffness. The M design variables are subject to upper and lower bounds,  $v_{i \max}$  and  $v_{i \min}$ , respectively.

A typical optimization method, applied to solve this problem, starts from a given design and continuously searches for better designs until it finds an optimum design. The trial designs along the path are of no value. The proposed method instead proceeds along a path of optimal designs for increasing amounts of resource  $\theta$ . The resource  $\theta$  is varied between the minimum  $\theta_{\min}$  required to satisfy the lower bound constraints and a maximum  $\theta_{\max}$  when all variables are at their upper bounds.

The path consists of several smooth segments, each segment being characterized by a set  $I_A$  of variables which are at their upper or lower bounds. Along each segment, some inequality constraints can be treated as equality constraints

$$v_j = v_{j \min}$$
 or  $v_j = v_{j \max}$  for  $j \in I_A$ , (2)

so that these variables can be eliminated from the optimization problem, while the other variables do not have to be constrained. The optimization problem along a segment can, therefore, be written as

$$\max_{v_i} \min_{u} \frac{u^t K u}{u^t K_G u} \quad \text{for } i \not \subseteq I_A ,$$
 (3)

such that  $c^{t}v - \theta = 0$ .

The solution of the problem consists of three related problems: solving the optimization problem along a segment, locating the end of the segment where the set  $I_A$  changes, and

# 3. Stationary equations along a segment and the homotopy method

## 3.1. Stationary conditions

It is common practice to normalize the displacement vector u such that the denominator of Rayleigh's quotient is unity and to treat this as an equality constraint. Then, using Lagrange multipliers  $\eta$  and  $\mu$ , the augmented function  $P^*$  is formed:

$$P^* = u^{t} K u - \eta [u^{t} K_{G} u - 1] - \mu [c^{t} v - \theta].$$
(4)

The following stationary conditions are obtained by taking the first derivative of  $P^*$  with respect to  $v_i$ , u,  $\eta$ , and  $\mu$ , and setting it equal to zero. (i) Optimality conditions:

$$u^{t} \frac{\partial K}{\partial v_{i}} u - \eta u^{t} \frac{\partial K_{G}}{\partial v_{i}} u - \mu c_{i} = 0 \quad \text{for } i \not \in I_{A}.$$

$$(5)$$

(ii) Stability conditions:

$$Ku - \eta K_{G}u = 0. (6)$$

(iii) Normalization constraint:

$$1 - u^t K_G u = 0 (7)$$

(iv) Total resource constraint:

$$\theta - c^{t}v = 0. \tag{8}$$

Equations (5)-(8) form a system of nonlinear equations to be solved for  $v_i$ , u,  $\eta$ , and  $\mu$ . A homotopy method is used to find the solutions of these equations as a function of  $\theta$ .

In certain ranges of structural resources, the optimal solution is known to be bimodal, i.e., the lowest buckling load is a repeated eigenvalue. The formulation for bimodal solutions is given in Appendix A. The existence of bimodal solutions also introduces additional transitions (bimodal to unimodal and vice versa) along the path of optimum solutions.

# 3.2. Homotopy method

The system of equations with a homotopy parameter  $\theta$  has the form

$$F(x, \theta, d) = 0, (9)$$

where  $\theta$  is a positive real number, F, x, and d are N-dimensional vectors, and N is the number of degrees of freedom. Note that F is viewed as a function of x (the design vector),  $\theta$  (the resource parameter), and d (the parameter vector, usually a random imperfection; see, e.g., [9]). The theoretical basis for globally convergent homotopy algorithms is the following fact from differential geometry [1].

THEOREM 3.1. Suppose that the  $N \times (2N+1)$  Jacobian matrix of F has full rank on

$$F^{-1}(0) = \{(x, \theta, d) \mid F(x, \theta, d) = 0, \, \theta_a < \theta < \theta_b\} .$$

Then for almost all N-vectors d (i.e., except those in a set of Lebesgue measure zero), the  $N \times (N+1)$  Jacobian matrix of

$$\tilde{F}(x, \theta) = F(x, \theta, d)$$

also has full rank on

$$\tilde{F}^{-1}(0) = \{(x, \theta) \mid \tilde{F}(x, \theta) = 0, \, \theta_a < \theta < \theta_b\}.$$

Alternatively, if d were picked at random, it is virtually always true that the Jacobian matrix has full rank on the solution set of

$$\tilde{F}(x,\,\theta) = 0\;. \tag{10}$$

According to the theory in [1], this full rank of the Jacobian matrix implies that the zero set of equations (10) contains a smooth curve  $\Gamma$  in (N+1)-dimensional  $(x, \theta)$  space, which has no bifurcations and is disjoint from other zeros of (10). The curve  $\Gamma$  can be parameterized by the arc length s as

$$x = x(s) , \qquad \theta = \theta(s) . \tag{11}$$

Taking the derivative of (10) with respect to arc length, the nonlinear system of equations is transformed to a set of ordinary differential equations

$$\left[\tilde{F}_{x}(x(s), \theta(s)), \tilde{F}_{\theta}(x(s), \theta(s))\right] \begin{bmatrix} \frac{\mathrm{d}x}{\mathrm{d}s} \\ \frac{\mathrm{d}\theta}{\mathrm{d}s} \end{bmatrix} = 0,$$
(12)

and

where  $\tilde{F}_x$  and  $\tilde{F}_{\theta}$  denote the partial derivatives of  $\tilde{F}$  with respect to x and  $\theta$ , respectively. With

$$x(0) = x_0$$
,  $\theta(0) = \theta_a$ , (14)

(12)-(14) can be treated as an initial value problem. We have thus converted the system of equations (9), parameterized by the vector d, to the initial value problem (12)-(14) whose trajectory gives the path of optimal solutions x. This technique differs significantly from standard continuation, imbedding, or incremental methods in that the resource parameter,  $\theta$ , is a dependent variable which can both increase and decrease along the path  $\Gamma$ . Also, no attempt is made to invert the Jacobian matrix  $\tilde{F}_x$  so that limit points pose no special difficulty. It differs from initial value or parameter differentiation methods also, since arc length s, rather than  $\theta$ , is the controlling parameter. The homotopy method is similar in spirit to the Riks-Wempner [12, 13] and Crisfield [14] methods, but the supporting mathematical theory and implementation details are very different, and the emphasis is on ordinary differential equation techniques rather than a Newton-type iteration.

The homotopy method as described in [1-10] is intended to solve a *single* nonlinear system of equations, and to converge from an arbitrary starting point with probability one. In this context  $\theta \in [0, 1]$ , and the zero curve  $\Gamma$  is bounded and leads to the (single) desired solution at  $\theta = 1$ . The d vector, viewed as an artificial perturbation of the problem, plays a crucial role. In the version of the method employed here,  $\theta \in (\theta_a, \theta_b)$ , each point along  $\Gamma$  has physical significance, and d is fixed at zero (no perturbation). Because d is not random, the claimed properties for  $\Gamma$  hold only in subintervals  $(\theta_a, \theta_b)$  of  $[0, \infty)$ . Detecting and dealing with these subinterval transition points is the essence of the modification of the homotopy method used

There are several approaches to tracking the curve  $\Gamma$ , which along with theoretical background can be found in [15]. A software package, HOMPACK, which implements several different homotopy algorithms, is under development at Sandia National Laboratories, General Motors Research Laboratories, Virginia Polytechnic Institute and State University, and the University of Michigan. One of the HOMPACK subroutines, FIXPNF, is used in the

# 4. Switching from one segment to the next

There are four types of events which end a segment and start a new one:

Type 1: a bound constraint becoming active (i.e., being satisfied as an equality);

Type 2: a bound constraint becoming inactive;

Type 3: transition from a unimodal solution to a bimodal solution;

Type 4: transition from a bimodal solution to a unimodal solution.

To switch from one segment to the next, we first need to locate the transition point. At a transition point there are a number of solution paths which satisfy the stationary equations, and we need to choose the optimum path.

#### 4.1. Locating the transition points

Transition points are located by checking the bound constraints and the optimality conditions.

The bound constraints

$$v_{i \min} \leq v_i \leq v_{i \max} \quad \text{for } i = 1, \dots, M$$
 (15)

are checked to detect a transition point of Type 1.

Optimality of the solution is checked by the Kuhn-Tucker conditions and the second-order conditions discussed below. The solution satisfies the Kuhn-Tucker conditions when all Lagrange multipliers are nonnegative. So a transition of Type 2 is detected by checking the positivity of the Lagrange multipliers associated with the bound constraints. These multipliers are obtained by adding the bound constraints to the formultion (3) and replacing the augmented function  $P^*$  by

$$P^* = u^{t} K u - \eta [u^{t} K_{G} u - 1] - \mu [c^{t} v - \theta] - \sum_{i \in I_A} \lambda_{1i} [v_{i \min} - v_{i}] - \sum_{i \in I_A} \lambda_{2i} [v_{i} - v_{i \max}].$$
(16)

Taking the first derivative of  $P^*$  with respect to  $v_i$  gives

$$u^{t} \frac{\partial K}{\partial v_{i}} u - \eta u^{t} \frac{\partial K_{G}}{\partial v_{i}} u - \mu c_{i} + \lambda_{1i} - \lambda_{2i} = 0 \quad \text{for } i \in I_{A}.$$

$$(17)$$

Since  $\lambda_{1i}$  is 0 for  $v \neq v_{i \min}$  and  $\lambda_{2i}$  is 0 for  $v_i \neq v_{i \max}$  for the above equations,  $\lambda_{1i}$  and  $\lambda_{2i}$  are given by

$$\lambda_{1i} = -u^{t} \frac{\partial K}{\partial v_{i}} u + \eta u^{t} \frac{\partial K_{G}}{\partial v_{i}} u + \mu c_{i} \quad \text{for } v_{i} = v_{i \min},$$

$$\lambda_{2i} = u^{t} \frac{\partial K}{\partial v_{i}} u - \eta u^{t} \frac{\partial K_{G}}{\partial v_{i}} u - \mu c_{i} \quad \text{for } v_{i} = v_{i \max}.$$
(18)

A Type-2 transition is detected by a Lagrange multiplier becoming nonpositive. Similar equations for the bimodal case are given in Appendix A.

The bimodal formulation replaces  $\eta$  by  $\eta_1$  and  $\eta_2$ , which are the Lagrange multipliers for the normalization constraints on the two buckling modes. When one of them becomes negative, the corresponding mode should be removed for the optimum design, so that we have a transition of Type 4 from bimodal to unimodal design.

For a transition of Type 3, we need to check if there is another buckling mode associated with a lower buckling load. This can be accomplished by checking the second-order optimality conditions for the buckling mode variables u given by

$$r^{t}[\nabla_{u}^{2}P^{*}]r > 0$$
 for every  $r$  such that  $\nabla_{u}h^{t}r = 0$ , (19)

where

$$[\nabla_u^2 P^*] = \left[\frac{\partial^2 P^*}{\partial u_s \, \partial u_t}\right], \qquad \nabla_u h = \left\{\frac{\partial h}{\partial u_s}\right\}, \qquad h = u^{\mathsf{t}} K_{\mathsf{G}} u - 1.$$

Alternatively we can solve the buckling problem (6) for the current design and check whether the buckling load obtained from the stationary conditions is truly the lowest one. The transition of Type 3 is detected by checking if

$$p \neq p_1 , \tag{20}$$

where p is the buckling load obtained from the stationary conditions while  $p_1$  is the first buckling load obtained by solving the stability conditions (6) for the given structure.

## 4.2. Choosing an optimum path

Once a transition point is located, we need to choose a path which satisfies the optimality conditions. Choosing an optimum path constitutes finding a set of active bound constraints for Type-1 and -2 transitions and the correct buckling modes for Type-3 and -4 transitions. These are obtained by using the Lagrange multipliers of the previous path and the sensitivity calculation on the buckling load. The procedure is explained separately for each type of transition.

A Type-1 transition occurs when one of design variables,  $v_i$ , hits the upper or lower bound. Then  $v_i$  is set at  $v_{i \max}$  or  $v_{i \min}$  and treated as a constant value. The number of design variables is reduced by one.

At a Type-2 transition, one of the Lagrange multipliers for the bound constraints,  $\lambda_{1i}$  and  $\lambda_{2i}$ , is found to be negative. The bound constraint corresponding to the negative  $\lambda_{1i}$  and  $\lambda_{2i}$  is set to be inactive and the number of design variables is increased by one.

At a transition from a unimodal solution to a bimodal solution (a Type-3 transition), the formulation requires two buckling modes,  $u_1$  and  $u_2$ , for the solution of the upcoming bimodal path. These modes can be obtained by solving the stability conditions (6) of the previous unimodal formulation, since the stability conditions give two buckling modes at the bimodal transition point.

At a transition from a bimodal to a unimodal solution (a Type-4 transition), two buckling modes are given from the bimodal solution. One of the Lagrange multipliers for the normalization constraints,  $\eta$ , is known to be negative from the previous transition check, so the buckling mode corresponding to the positive  $\eta$  is chosen.

Some of the above transitions can occur simultaneously. Special treatment is required in certain cases where the Lagrange multipliers are not available. In general, the optimum design requires at least one design variable  $v_i$  for a unimodal case and two design variables for a bimodal case. At a Type-1 transition, the number of design variables is reduced by one, and at a Type-3 transition the bimodal formulation requires one more design variable in case the previous unimodal path has only one design variable. So some Type-1 or Type-3 transitions occur simultaneously with a Type-2 transition which allows an additional design variable. In that case, the Lagrange multipliers  $\lambda_{1i}$  and  $\lambda_{2i}$ , which are used at a Type-2 transition to determine a new design variable, are not available. We then rely on the sensitivity information of p with respect to v. For a unimodal case, the location of the new design variable  $v_i$  is

determined where  $\mathrm{d}p/\mathrm{d}\theta$  is maximized. For a bimodal case, we need to find a combination of i and j which maximizes the value of the bimodal buckling load for a small increment of the total available resource. Considering the bound constraints in the formulation, the new design variables are determined by

$$\max_{i,j} \frac{\mathrm{d}p}{\mathrm{d}\theta} = \frac{\partial p_1}{\partial v_i} \frac{\mathrm{d}v_i}{\mathrm{d}\theta} + \frac{\partial p_1}{\partial v_j} \frac{\mathrm{d}v_j}{\mathrm{d}\theta} \,,$$
 such that 
$$\frac{\partial p_1}{\partial v_i} \frac{\mathrm{d}v_i}{\mathrm{d}\theta} + \frac{\partial p_1}{\partial v_j} \frac{\mathrm{d}v_j}{\mathrm{d}\theta} = \frac{\partial p_2}{\partial v_i} \frac{\mathrm{d}v_i}{\mathrm{d}\theta} + \frac{\partial p_2}{\partial v_j} \frac{\mathrm{d}v_j}{\mathrm{d}\theta} \,,$$
 
$$\frac{\mathrm{d}v_i}{\mathrm{d}\theta} \ge 0 \quad \text{for } v_i = v_{i\,\mathrm{min}} \,,$$
 
$$\frac{\mathrm{d}v_i}{\mathrm{d}\theta} \le 0 \quad \text{for } v_j = v_{j\,\mathrm{min}} \,,$$
 
$$\frac{\mathrm{d}v_j}{\mathrm{d}\theta} \ge 0 \quad \text{for } v_j = v_{j\,\mathrm{min}} \,,$$
 
$$\frac{\mathrm{d}v_j}{\mathrm{d}\theta} \le 0 \quad \text{for } v_j = v_{j\,\mathrm{max}} \,,$$

where  $p_1$  and  $p_2$  are the buckling loads corresponding to the buckling modes  $u_1$  and  $u_2$ , respectively.

After we obtain the design variables v and the buckling modes u, we need the Lagrange multipliers  $\mu$ ,  $\eta$ , and  $\gamma$  at the transition point to complete the set of starting values for the next solution path. These are obtained by solving the stationary conditions for the given u and v. For example, in the unimodal case,  $\eta$  is obtained from the stability conditions (6) and  $\mu$  is obtained by solving one of the optimality conditions (5).

#### 5. Example problem

The example used to demonstrate the proposed procedure is a simply supported column on an elastic foundation taken from [11].

The design problem is to find the optimum distribution of the foundation to maximize the lowest buckling load. The design variable is the foundation stiffness. The column is modeled by sixteen beam finite elements and the foundation stiffness for each element is assumed to be constant. The geometry of the column and the foundation is shown in Fig. 1. Because of the symmetry of the problem, the foundation distribution is assumed to be symmetric, so there are eight design variables,  $K_1, \ldots, K_8$ . The constraint of the total foundation stiffness is given by

$$\frac{1}{8} \sum_{i=1}^{8} K_i = K_{\rm T} \,, \tag{22}$$

where  $K_{\rm T}$  is the total foundation stiffness used as the homotopy parameter.

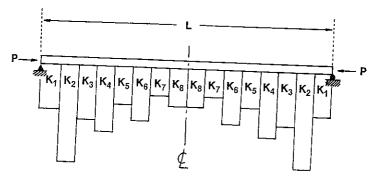


Fig. 1. Geometry of column and foundation.

The upper and lower bound constraints are given by

$$K_{\min} \le K_i \le K_{\max}$$
 for  $i = 1, \dots, 8$ ,

where  $K_{\min}$  is the lower bound and  $K_{\max}$  is the upper bound of the foundation stiffness. The buckling load P and the foundation stiffness parameters are expressed in nondimensional form as

$$p = \frac{PL^{2}}{EI}, k_{i} = \frac{K_{i}L^{4}}{EI}, k_{\min} = \frac{K_{\min}L^{4}}{EI}, k_{\max} = \frac{K_{\max}L^{4}}{EI},$$

$$k_{T} = \frac{K_{T}L^{4}}{EI}, (24)$$

where EI is the bending stiffness of the column. The lower bound  $k_{\min}$  is set at 0 and the upper bound  $k_{\max}$  is set at 20,000. The procedure starts with a uniform column without any foundation material (the total nondimensional foundation stiffness  $k_{\mathrm{T}}$  is zero) and optimum designs are obtained for values of  $k_{\mathrm{T}}$  up to 20,000.

Figure 2 shows the buckling loads corresponding to optimum designs obtained for  $0 \le k_T \le 20,000$ . This curve has 18 transition points and consists of 19 solution paths denoted by the letters A-S. The circles on the curve indicate the transition points and the dots are the solutions traced along the optimum path. The solutions on the first path A and the last path S are unimodal and the other solutions are bimodal. This is due to the fact that the starting point of  $k_T = 0$  and the last point of  $k_T = 20,000$  are uniform designs (with unimodal solutions) in which foundations are all at the lower or at the upper bound. The buckling loads for a uniform foundation are also shown in Fig. 2 (dashed line). Note that the two curves meet at the last point where all design variables are at their upper bound and the only feasible design is uniform.

One point from each path in Fig. 2 is selected, and the optimum foundation distribution and corresponding buckling mode for these points are shown in Fig. 3.

At the starting point of  $k_{\rm T}=0$ , the column has no foundation at all. So we need to find a column element at which the foundation is placed when we increase  $k_{\rm T}$ . Since Lagrange multipliers  $\lambda_{1i}$  and  $\lambda_{2i}$  are not available at this point, it is treated the same as if a Type-1 transition occurs simultaneously with a Type-2 transition. For this example, a foundation is initially placed at the midspan where  ${\rm d}p/{\rm d}k_{\rm T}$  is maximum.

The unimodal solution becomes bimodal at the transition point AB from path A to path B

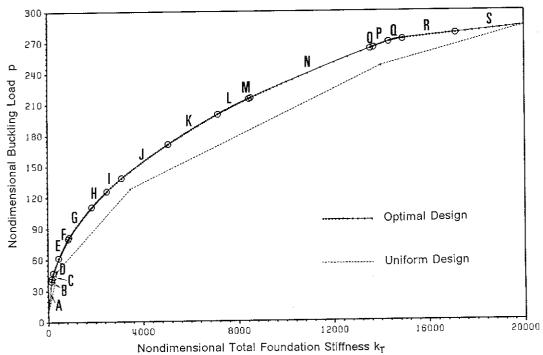


Fig. 2. Buckling load versus the total foundation stiffness.

(this is a Type-3 transition). This requires one more design variable because the previous unimodal path has only one design variable (a Type-2 transition occurs at the same time). At transition points BC, CD, DE, and EF, one of the foundation stiffnesses becomes zero (the lower bound) and another foundation stiffness becomes nonzero. Each of these points is a simultaneous transition of Types 1 and 2 in the bimodal solution, requiring the solution of (21). At transition points FG, GH, IJ, JK, MN, OP, and QR, new variables become nonzero. These are Type-2 transitions where the lower bound constraint becomes inactive. At transition points HI, KL, LM, NO, and PQ, one of the foundation stiffnesses hits the lower or upper bound. These are Type-1 transitions. The last transition (RS) is a Type-4 transition at which the bimodal solution becomes unimodal.

Most of the computational effort of tracing the optima is associated with the evaluation of the Jacobian matrix. The curve of Fig. 2 required about 200 integration steps to trace, each requiring 1 to 3 (mostly 1) Jacobian evaluations. The Jacobian was evaluated numerically, using forward finite differences.

#### 6. Concluding remarks

A typical optimization method starts from a given design and continuously searches for better designs until it finds an optimum design. The trial designs along the path are of no value. In this paper, a strategy for tracing a path of optimum solutions parameterized by an amount of available resources was discussed. Equations for the optimum path were obtained using Lagrange multipliers, and were solved by a homotopy method.

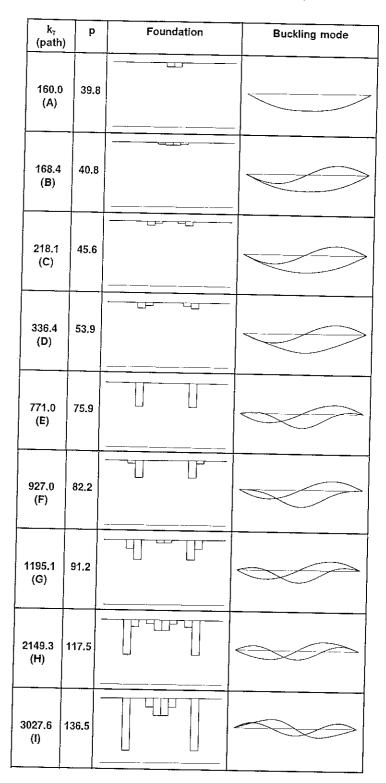


Fig. 3. Optimum foundation designs.

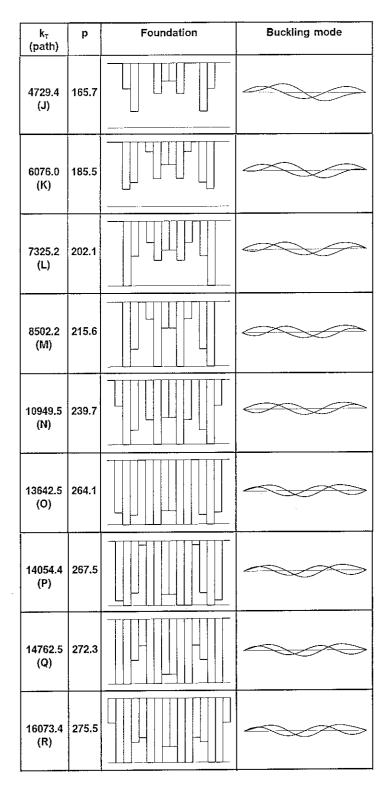


Fig. 3 (cont.). Optimum foundation designs.

k <sub>T</sub> (path)	Р	Foundation	Buckling mode	
17858.0 (S)	279.7			

Fig. 3 (cont.). Optimum foundation designs.

The solution path has several branches due to changes in the active constraint set and transition from unimodal to bimodal solutions. The Lagrange multipliers and the second-order optimality conditions were used to detect branching points and to switch to the optimum

The procedure was applied to the design of a foundation which supports a column for maximum buckling load. The total available foundation was used as a homotopy parameter. Starting from a minimum foundation which satisfies the lower bound (in this example it is zero), a set of optimum foundation designs was obtained for the full range of total foundation stiffness (from zero to the upper bound).

#### Appendix A. Bimodal formulation

To seek the solutions with double eigenvectors, the problem is to be formulated assuming bimodality of solutions, or equality of the two lowest eigenvalues,  $P_1$  and  $P_2$ . They are expressed in terms of the Rayleigh quotient

$$P_i = \frac{u_i^t K u_i}{u_i^t K_G u_i} \quad \text{for } i = 1, 2,$$

where  $u_i$  are the corresponding eigenvectors.

Treating the bimodality condition as an equality constraint,  $P_1 - P_2 = 0$ , the augmented function  $P^*$  is formed

$$P^* = u_1^t K u_1 - \gamma [u_1^t K u_1 - u_2^t K u_2] - \sum_{i=1}^2 \eta_i [u_i^t K_G u_i - 1] - \mu [c^t v - \theta].$$

The stationary conditions are obtained by taking the first derivatives of  $P^*$  with respect to  $v_i, u, \gamma, \eta_1, \eta_2$ , and  $\mu$  and setting them to zero. Thus we obtain:

(i) Optimality conditions:

$$(1-\gamma)u_1^t \frac{\partial K}{\partial v_i} u_1 + \gamma u_2^t \frac{\partial K}{\partial v_i} u_2 - \eta_1 u_1^t \frac{\partial K_G}{\partial v_i} u_1 - \eta_2 u_2^t \frac{\partial K_G}{\partial v_i} u_2 - \mu c_i = 0 \quad \text{for } i \not \in I_A .$$

(ii) Stability conditions:

$$(1-\gamma)Ku_1 - \eta_1K_Gu_1 = 0$$
,  $\gamma Ku_2 - \eta_2K_Gu_2 = 0$ .

(iii) Bimodality constraint:

$$u_2^{t} K u_2 - u_1^{t} K u_1 = 0 .$$

(iv) Normalization constraints:

$$1 - u_1^{\mathsf{t}} K_{\mathsf{G}} u_1 = 0 \; , \qquad 1 - u_2^{\mathsf{t}} K_{\mathsf{G}} u_2 = 0 \; .$$

(v) Total resource constraint:

$$\theta - c^{\mathsf{t}} v = 0 .$$

The Lagrange multipliers for the bound constraints,  $\lambda_{1i}$  and  $\lambda_{2i}$ , are required for the transition check. These are obtained by adding the bound constraints to the augmented function  $P^*$  and taking the first derivatives of  $P^*$  with respect to  $v_i$ . They are given by

for  $v_i = v_{i \text{ max}}$ .

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