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Abstract

Design optimization of finite element-based structures can be very compute intensive thus inhibiting interactive design. The research presented here outlines a fast method for approximating eigenvalues and eigenvectors across a wide range of design changes. An optimization scheme is described that combines Padé Approximants with curve-fitting techniques to achieve good approximations for large design changes.

Disciplines

Computer-Aided Engineering and Design

APPROXIMATING EIGENVALUES AND EIGENVECTORS USING PADÉ APPROXIMANTS

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ABSTRACT

Design optimization of finite element-based structures can be very compute intensive thus inhibiting interactive design. The research presented here outlines a fast method for approximating eigenvalues and eigenvectors across a wide range of design changes. An optimization scheme is described that combines Padé Approximants with curve-fitting techniques to achieve good approximations for large design changes.

INTRODUCTION

Finite element-based optimization typically uses finite element calculations as part of the objective function. The challenges to the use of such an optimization are the formulation of the finite element problem and the objective function based on the results of that problem. Included in the selection of the objective function are choices of design parameters, and the limits on these parameters in the form of design constraints. Constraints such as maximum weight or maximum stress may also be indirectly based on the design parameters or on the finite element results. Determining constraints is often a subjective exercise dependent on the skill and prior experiences of the designer.

Once the problem formulation is complete, the optimization software takes the formulation and calculates the optimum design. In essence, the optimization software acts as a "black box" operation independent of the designer. If the designer is not pleased with the outcome of the optimization, the objective function is adjusted and the optimization repeated. For large degree-of-freedom systems, each optimization run may take several hours or even days.

Our overall goal is to develop software that facilitates the interactive participation of the designer in the optimization process. An important part of this software is the use of approximations to re-

duce the computational burden required for each of several minimizations of objective functions that will be inherent in the designer's interactive participation in the process. Our approach is to develop high speed approximations of the finite element solutions for use in the objective function.

In the design of systems where vibration characteristics are of interest, the objective function often involves natural frequencies. The natural frequencies derive from eigenproblems of the form

$$K(e)U(e) = \lambda M(e)U(e) \quad (1)$$

Equation (1) indicates that the natural frequencies or eigenvalues (λ), the mode shapes or eigenvectors (U), the stiffness terms (K), and the mass terms (M) are functions of the design variable e . Often, obtaining solutions to equation (1) for large degree-of-freedom systems is very compute intensive, and further, many solutions may be required in the optimization process. This presents a challenge which may preclude interactive optimization on commonly available workstations. The research presented here focuses on developing fast approximation methods for natural frequencies and mode shapes to facilitate interactive optimization.

APPROXIMATIONS FOR SINGLE DESIGN VARIABLE PROBLEMS

In 1968 Fox and Kapoor suggested using linear Taylor series of the form

$$\lambda(e + \Delta e) = \lambda(e) + \frac{\delta \lambda}{\delta e}(\Delta e) \quad (2)$$

$$U(e + \Delta e) = U(e) + \frac{\delta U}{\delta e}(\Delta e) \quad (3)$$

to approximate eigenvalues and eigenvectors as a function of a single design change. This spawned research into various methods of calculating eigenvalue and eigenvector derivatives. Surveys of these methods are presented by Adelman and Haftka (1986) and Murthy and Haftka (1987).

Since λ and U are rarely linear with respect to the design parameter e , a nonlinear Taylor series may be a useful approximation. Rizai and Bernard (1987) used this approach to approximate eigenvalues and eigenvectors of a beam, where n derivatives are needed for the series:

$$\lambda(e + \Delta e) = \lambda(e) + \sum_{j=1}^n \frac{\delta^j \lambda}{\delta e^j} (\Delta e)^j \quad (4)$$

$$U(e + \Delta e) = U(e) + \sum_{j=1}^n \frac{\delta^j U}{\delta U^j} (\Delta e)^j \quad (5)$$

EIGENVALUE AND EIGENVECTOR DERIVATIVES

The efficient calculation of eigenvalue and eigenvector derivatives is essential to the development of fast approximations. Whitesell (1984) introduced a method to calculate these derivatives which takes advantage of the properties of the generalized inverse of a matrix, in this case $(K - \lambda_m M)^{-1}$. This method allows calculation of the derivatives in $O(n^2)$ calculations. The expression for the i^{th} derivative of the m^{th} eigenvalue and the m^{th} eigenvector with respect to design variable e , where:

$$\frac{d^i \lambda_m}{d e^i} = i! \lambda_m^{(i)} \quad (6)$$

$$\frac{d^i U_m}{d e^i} = i! U_m^{(i)} \quad (7)$$

is:

$$\lambda_m^{(i)} = U_m^T y^{(i)} \quad (8)$$

$$U_m^{(i)} = - (K - \lambda_m M)^{-1} y^{(i)} + C_i U_m \quad (9)$$

The common term in equations (8) and (9) is $y^{(i)}$, which can be calculated as follows:

$$y^{(i)} = \sum_{j=0}^{i-1} K^{(i-j)} U_m^{(j)} - \sum_{j=0}^{i-1} \left(\sum_{\substack{k=0 \\ k \neq i}}^{i-1} M^{(i-j-k)} \lambda_m^{(k)} \right) U_m^{(j)} \quad (10)$$

The C_i term in the eigenvector derivative equation is:

$$C_i = -\frac{1}{2} \left[\left(\sum_{k=1}^i U_m^{(i-k)T} M^{(k)} \right) U_m + \sum_{j=1}^{i-1} \left(\sum_{k=0}^{i-j} U_m^{(i-j-k)T} M^{(k)} \right) U_m^{(j)} \right] \quad (11)$$

Embedded within both equations (10) and (11) are n derivatives of the mass and stiffness matrices, M and K . Since analytical derivatives of these matrices are generally not available from the finite element model, Bernard, Kwon and Wilson (1990) have shown that cubic approximations to elements in the matrices are sufficient for calculating eigenvalue and eigenvector derivatives.

APPROXIMATIONS FOR MULTI-DESIGN VARIABLE PROBLEMS

In large systems, there are generally several design variables of interest. Since computing an approximation using a nonlinear Taylor series involving several variables will contain many cross-derivatives that are very difficult to obtain, Rizai and Bernard (1987) proposed a two-step optimization scheme to allow for optimization of a design with many design variables. The first step uses a linear Taylor series to approximate the eigenvalues and eigenvectors. This series is made up of the linear approximations of each of the s design variables.

$$\lambda(e + \Delta e) = \lambda(e) + \sum_{k=1}^s \frac{\delta \lambda}{\delta e_k} (\Delta e_k) \quad (12)$$

This first step produces an optimum set of design parameters, \bar{e} , based on the linear approximation to the finite element results. If the problem is linear with respect to the design changes, then the optimum solution has been found.

If the problem is nonlinear, then the assumption is made that the optimum design, e_{opt} , will be a scalar multiple, ϵ , of the design changes found in the previous linear optimization.

$$e_{opt} = \epsilon \bar{e} \quad (13)$$

The problem is reformulated in terms of optimization with respect to one parameter: the scalar multiple, ϵ . A nonlinear Taylor series in the one scalar parameter can be used in the final step of the optimization. However, Taylor series approximations which include higher-order terms of the series can experience convergence difficulties. The usual approach to overcoming this difficulty is to re-solve the eigenvalue problem at the point where lack of convergence is detected. This paper presents a method targeted at improving the single-variable approximation needed in the second step of the multi-design variable optimization technique presented by Bernard and Rizai.

COMBINING PADÉ APPROXIMANTS WITH CURVE-FITTING TECHNIQUES

In 1989 Vance and Bernard presented a method that used a fifth-order polynomial curve-fit to approximate eigenvalues across a wide design range. In 1992, they expanded the method by combining nonlinear Taylor series approximations with curve-fit techniques (Vance and Bernard, 1992). Based on information at the initial design point, a nonlinear Taylor series was formed for the eigenvalue. At the design value where the Taylor series exhibited signs of divergence, a re-solve of the eigenvalue problem was performed. Once new solutions were obtained, local derivatives were calculated and used to form a polynomial between the re-solve point and the previous design point. The process was repeated until the entire design range had been covered with polynomial curve-fits.

One difficulty encountered when using curve-fit techniques occurs when the system possesses a repeated eigenvalue within the design range. This causes the eigenvalues to be reordered at the end of the range. Vance and Bernard (1992) proposed using inner product matching to identify the correct endpoint eigenvalue to use in the curve-fit.

Inner product matching is based on the mass-orthogonality properties of eigenvectors. Once divergence of the Taylor series indicates the need for a re-solve, a Taylor series estimate of the eigenvector at the re-solve point (U_{est}) is calculated using equation (5) with derivatives from equation (9). (Note that the eigenvector derivatives would already be available since they were needed to calculate the eigenvalue derivatives.) New eigenvectors, U_r , are obtained at the re-solve point through solution of the eigenvalue problem (equation (1)). The inner product matching criteria is applied as follows.

$$\text{If } |U_{est}^T M_r U_r| \cong 1.0$$

$$\text{then } U_{est}^T \text{ is the match to } U_r.$$

U_{est}^T is multiplied by successive eigenvectors U_r from other modes until equation (7) is satisfied.

Another difficulty encountered when using the Taylor series/curve-fit method is when the eigenvalue of interest possesses several poles within the design range. These poles cause the Taylor series to diverge, resulting in the need for several re-solves in order to get a good approximation for the eigenvalues and eigenvectors across the design range. Since the intent is to reduce the redesign time, it is important to limit the number of re-solves in the design range.

The research presented here replaces the nonlinear Taylor series with a Padé Approximant of similar degree. This allows the initial approximation to be made for larger design changes before divergence is detected. The result is that fewer re-solves are needed within the design range.

PADÉ APPROXIMANTS

Whitesell (1984) presented a method for using Padé Approximants in structural design reanalysis to overcome the convergence difficulties of higher-order power series. Padé Approximants are rational functions which often show superior convergence properties over higher-order power series (Brezinski, 1991). When the eigenvalue can be expressed in the form of equation (4) then the Padé Approximant, $R_{l,m}$, for the eigenvalue is

$$R_{l,m} = \frac{P}{Q} \cong \lambda(e + \Delta e) \quad (14)$$

where P is an l^{th} order polynomial in Δe and Q is an m^{th} order polynomial in Δe .

There are many methods that can be used to find the Padé Approximant of a series (Brezinski, 1991). The method used here is from Whitesell (1984). The Padé Approximant $R_{l,m}$, can be calculated as follows:

$$R_{l,m} = \sum_{i=0}^m \frac{1}{\eta_i} \quad (15)$$

The η_i are the solution to the following linear equations:

$$H\tau = p \quad (16)$$

$$H = \begin{bmatrix} h_l & h_{l-1} & \dots & h_{l-m} \\ h_{l+1} & h_l & \dots & h_{l-m+1} \\ \dots & \dots & \dots & \dots \\ h_{l+m} & h_{l+m-1} & \dots & h_l \end{bmatrix} \quad (17)$$

$$\tau = [\eta_1 \ \eta_2 \ \eta_3 \ \dots \ \eta_m]^T \quad (18)$$

$$p = [1 \ 1 \ 1 \ \dots \ 1]^T \quad (19)$$

Each h_i term is the i^{th} partial sum of the Taylor series expression for the eigenvalue (equation (4)). As can be seen from equation (17), the largest derivative needed for the $R_{l,m}$ Padé Approximant is the $l+m$ derivative.

The method illustrated in the next section involves using a combination of Padé Approximants and polynomial curve-fits. Given the solution to the eigenproblem at the initial design value and a specified range for the acceptable design values, an approximation for the eigenvalue based on the initial design value is formed. As the design parameter is changed, the approximation is calculated

and a test for divergence is performed. At the design value where divergence of the approximation is detected, a re-solve of the eigenproblem is performed. An estimate of the eigenvectors is made and inner product matching is performed. Then a curve-fit is calculated for the design sub-range and the process is repeated until the entire design range has been spanned by polynomial curves.

PLATE EXAMPLE

The plate shown in Figure 1 is 1 meter square. Three-fourths of the plate is 1 mm thick. The design variable is the thickness of the remaining fourth of the plate which is initially set at 0.500 mm. The design range extends from 0.500 mm to 1.200 mm. A finite element model of the plate was made using SDRC's I-DEAS software. The model consists of 16 quadrilateral shell elements each with 8 nodes. All of the edges of the plate are fixed which resulted in 165 degrees-of-freedom. The modulus of elasticity is 2.067×10^3 MPa, the density is 7.820×10^3 kg/m³, and Poisson's ratio is 0.29. The eigenvalue and eigenvector solutions were obtained using MSC/NASTRAN software.

The ninth mode was selected as the mode of interest because, for this model, several poles exist within the design range selected. We chose to use a 4-term Taylor series since we have found in practice that nothing is gained at poles by using higher order terms in the series. We also chose to use a $R_{4,4}$ Padé Approximant because it proved to be the lowest order that gave sufficient convergence. Also note that the $R_{4,4}$ Padé is the ratio of two cubic power series.

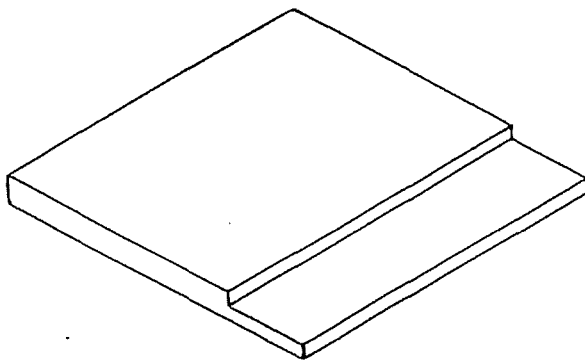


FIGURE 1: PLATE MODEL

Power Series Method

For the plate of Figure 1, derivatives of the ninth eigenvalue and eigenvector were calculated at $t = 0.500$ mm. Then a 3-term power series and a 4-term power series for the eigenvalue was formed us-

ing equation (4). This provided a continuous approximation of the eigenvalue for any given change in thickness. As the thickness was increased beyond the initial 0.500 mm, the values of both series were computed. The first indication of divergence of the 3-term power series occurred at $t = 0.648$ mm. A similar power series was formed for the eigenvector and an estimate of the eigenvector at $t = 0.648$ was made. A re-solve was performed at that design value and the inner product matching identified the 9th mode eigenvector as the match. Because six derivatives and two solutions were available, this allowed a seventh-order curve to be formed between the eigenvalues and eigenvectors at the two endpoints of the range.

Next, a power series for the eigenvalue was formed at $t = 0.648$ mm and testing for divergence continued, using larger design changes. For the sub-range starting at $t = 0.648$ mm, divergence occurred at $t = 0.922$ mm. A re-solve was performed at $t = 0.922$ mm, the eigenvector was estimated and the inner product matching performed. The 9th mode eigenvector was identified as the match to the estimated 9th mode eigenvector. Once again a seventh-order curve was formed between the two endpoints of the sub-range.

For the last part of the design range, the 3-term power series was able to approximate to the end of the design range without a re-solve. Because there is a repeated eigenvalue at $t = 1.000$ mm the eigenvalues switched order in the interval from $t = 0.922$ mm and $t = 1.200$ mm. The inner product matching correctly indicated that the 9th mode eigenvector at $t = 0.922$ mm matched the 10th mode eigenvector at $t = 1.200$ mm. Therefore a seventh-order curve was formed between the 9th eigenvalue at $t = 0.922$ mm and the 10th eigenvalue at $t = 1.200$ mm to complete the fit across the design range.

Figure 2 shows the 3-term and 4-term power series for the ninth mode eigenvalue across each sub-range. This figure illustrates how the series are starting to diverge before the divergence criteria of 5% is reached. The figure also shows the seventh-order curve-fits placed within each of the three sub-ranges: 0.500 mm to 0.648 mm, 0.648 mm to 0.922 mm, and 0.922 mm to 1.200 mm. Using the power series as an indicator of when to re-solve resulted in the need for three re-solutions across the design range. The seventh-order curve-fits provide a good approximation across the entire design range; however, the cost of this procedure is three re-solves and calculation of three derivatives at each of the three re-solve design values.

Padé Approximant Method

To compare the Padé method with the power series method an $R_{3,3}$ Padé and an $R_{4,4}$ Padé were formed at $t = 0.500$ mm to approximate the eigenvalue of the 9th mode as a function of thickness change. As the thickness was increased from 0.500 mm, the difference between the two eigenvalue approximations did not differ by more than 5% at any point within the design range. Therefore, only one re-solve at the end of the design range was required. The eigenvector approximation was calculated and used for inner product matching. The inner product matching correctly identified the 10th mode eigenvalue at $t = 1.200$ mm as the match to the 9th mode eigenvalue at the original design. The results are shown in Table 1.

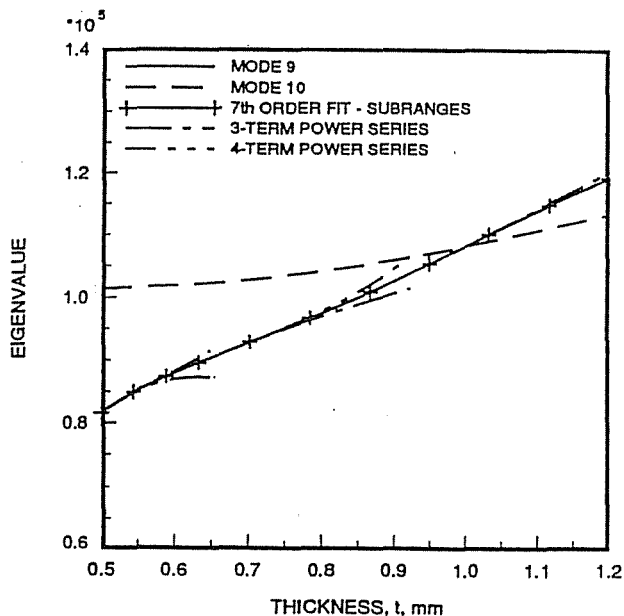


FIGURE 2: POWER SERIES APPROXIMATION OF THE NINTH MODE

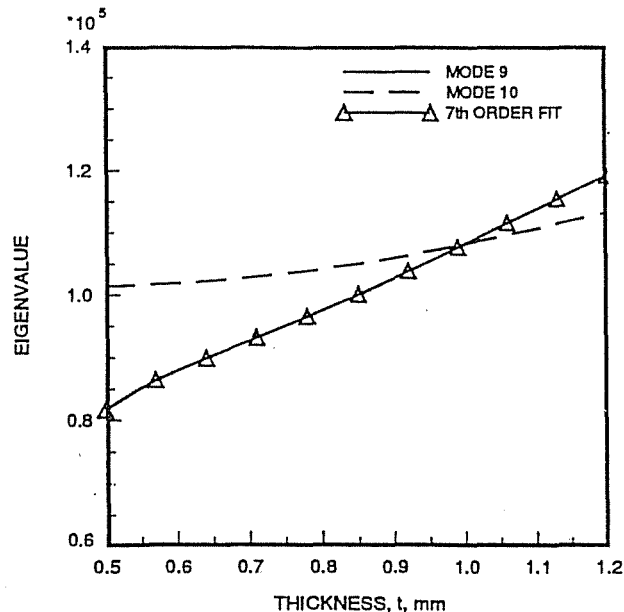


FIGURE 3: SEVENTH-ORDER CURVE-FIT ACROSS THE ENTIRE DESIGN RANGE

Table 1: MODE 9 INNER PRODUCT MATCHING

Inner Product with	at $t=1.200\text{mm}$
$M_r U_{r1}$	3.398×10^{-2}
$M_r U_{r2}$	8.382×10^{-9}
$M_r U_{r3}$	7.373×10^{-2}
$M_r U_{r4}$	1.863×10^{-9}
$M_r U_{r5}$	-7.466×10^{-2}
$M_r U_{r6}$	-1.210×10^{-1}
$M_r U_{r7}$	3.725×10^{-9}
$M_r U_{r8}$	6.985×10^{-2}
$M_r U_{r9}$	0.000
$M_r U_{r10}$	1.019

A seventh-order polynomial curve was calculated between $t = 0.500$ mm and $t = 1.200$ mm. Figure 3 shows the polynomial fit for the eigenvalue across the entire design range. Comparing Figure 2 to Figure 3 indicates that the power series approximation, which required three re-solves, was unnecessarily expensive because using a seventh-order curve-fit across the entire range was sufficient.

CALCULATION COSTS

The previous example was performed on a DECstation 3100 workstation using MSC/NASTRAN DMAP software for the eigenvalue derivative calculations. The Taylor series method required two re-solves within the design range while the Padé method was able to span the entire range without a re-solve. Table 2 presents a summary of the computation costs for the Taylor series method and the Padé method. The data in this table show that the Taylor series method took twice as long as the Padé method.

EIGENVECTOR APPROXIMATIONS

The Padé Approximant of the eigenvalue was used to determine where a re-solve should be calculated within the design range. Eigenvector approximations were used to perform inner product matching which identified the endpoints to be used in the polynomial curve-fit. Furthermore, the curve-fit for the eigenvectors, coupled with the increasing power of modern workstations, opens up exciting possibilities. In particular, since the eigenvector curve-fit can be calculated in real time, there exists the potential to display mode shapes as a function of a design parameter under the designer's control. Furthermore, the techniques presented here offer the potential to do finite element-based optimization interactively, facilitating an optimization procedure based on minimization of an objective function, assessment of the results using real time interactive display, re-formulation of the objective function via constraint changes, reassessment via real time display, etc. We believe this procedure, which is referred to as designer-weighted-optimization, has the potential to allow the designer to become a much more influential player in the optimization process.

Table 2: COMPUTATION TIME

Operation	Padé method	Taylor series
Initial solution	32.4 s	32.4 s
M and K derivatives	22.0 s	22.0 s
Derivative pre-process	21.5 s	21.5 s
Derivative calculations @2.3 s each	18.4 s	6.9 s
Re-solves	-	64.8 s
M and K derivatives	-	44.0 s
Derivative pre-process	-	43.0 s
Derivative calculations	-	13.8 s
End solution	32.4 s	32.4 s
End derivative pre-process	21.5 s	21.5 s
End derivative calculations	6.9 s	6.9 s
TOTAL	155.1 s	309.2 s

Vance, J.M. and Bernard, J.E. "Approximating Eigenvectors and Eigenvalues Across a Wide Range of Design." *Proceedings of the MacNeal-Schwendler 1992 World Users' Conference*, Dearborn, Michigan, May 1992, to be published in *Finite Elements in Analysis and Design*, 1993.

Vance, J.M. and Bernard, J.E. "Interactive Analysis of Vibration Modes Using Approximation Algorithms and Computer Graphics." *Computer-Aided Design*, 21, No. 7, 1989, 430-434.

Whitesell, J.E. "Rational Approximants in Structural Design Re-analysis." *Journal of Mechanisms, Transmissions, and Automation in Design*, 106, 1984, 114-118.

REFERENCES

Adelman, Howard M. and Raphael T. Haftka. "Sensitivity Analysis of Discrete Structural Systems." *AIAA Journal*, 24, No. 5, 1986, 823-832.

Bernard, J.E., Kwon, S.K. and Wilson, J.A., "Differentiation of Mass Stiffness Matrices for High Order Sensitivity Calculations in Finite Element-Based Equilibrium Problems." *Proceedings, ASME Design Automation Conference*, September 16-19, 1990, to be published in the *ASME Journal of Mechanical Design*.

Brezinski, Claude. *History of Continued Fractions and Padé Approximants*. Springer Series in Computational Mathematics 12, Springer Verlag, New York, 1991.

Fox, R.L. and Kapoor, M.P. "Rates of Change of Eigenvalues and Eigenvectors." *AIAA Journal*, 6, No. 12, 1968, 2426-2429.

I-DEAS Finite Element Modeling User's Guide, Version 5, Structural Dynamics Research Corporation, Milford, Ohio, 1990.

MSC/NASTRAN User's Manual, Version 66A, The MacNeal-Schwendler Corporation, Los Angeles, CA, November 1989.

Murthy, Durbha V. and Haftka, Raphael T. "Survey of Methods for Calculating Sensitivity of General Eigenproblems." Sensitivity Analysis in Engineering (symposium), NASA Langley Research Center, Hampton, VA, Feb. 1987. NASA CP-2457, NTIS N87-18867.

Rizai, Matt N. and Bernard, James E. "An Efficient Method to Predict the Effect of Design Modifications." *Journal of Mechanisms, Transmissions, and Automation in Design*, 109, 1987, 377-384.