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The Generalized Rayleigh Quotient Approximation as a Search Objective for SEM Pole Determination

by

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1. INTRODUCTION

The Singularity Expansion Method [1],[2] (SEM) provides a convenient means for characterizing the electromagnetic behavior of a body in the form of complex resonances and modal fields associated with these resonances. The representation is complete in the sense that the response of an object may be constructed for an arbitrary incident field and an arbitrary observation point.

Although conceptually simple, the task of determining the SEM quantities that describe a system can be very involved and time-consuming. For any but simple geometries the complex natural frequencies or "poles" are generally derived by means of iterative searching for the zeros of the determinant representing the discretized integral equation of the structure. These poles comprise the fundamental quantities in the SEM description. The Prony's method approach developed only recently by Van Blaricum and Mittra [3] provides an alternative technique but requires the knowledge of complete current distribution on the surface of the body due to some given transient excitation with a broad spectrum. This response may be derived either through an analytical or numerical solution of a mathematical model of the system or through measured response data. In the direct pole search procedure, we continue the mathematical operator equation into the complex frequency domain and

seek the complex resonant frequencies for which this operator equation has a homogeneous solution, cf. [2]. Either of these approaches embraces significant computational effort.

The high computational cost encountered in determining the SEM poles in the method of moments integral equation formulation is due to the fact that one seeks the complex zeros of a complex transcendental equation which is obtained by equating the determinant of a system matrix to zero. Typically, generating a single determinant value is a significant computation in itself. To date, most workers have used a classical numerical analysis approach such as Muller's method to seek out the zeros of the determinant. More recently, Baum, Singuraju and Giri have exploited the principle of the argument in complex variable theory in order to improve the search algorithms [4,5]. This approach, too, requires multiple calculations of the determinant of a moment matrix.

In this note we report a new approach to matrix zero searching which offers a significant computational gain over determinant calculations. The method utilizes two significant features of the moment-method-SEM approach, viz., (1) The approaching of zero by a matrix determinant is equivalent to an eigenvalue of the matrix approaching zero; and (2) Good estimates of the eigenvector and biorthogonal vector associated with this zero eigenvalue are

available by way of only two determinant evaluations. These evaluations may be at an arbitrary point within a relatively large neighborhood of the pole. The two estimated vectors may then be used in conjunction with the moment matrix evaluated for any location in a generalized Rayleigh quotient. This constitutes a variational form for the appropriate eigenvalue at that complex frequency. This eigenvalue can be used as the zero search objective for either a classical zero search method or for the argument number method of references [4] and [5].

2. RELATIONSHIP OF SEM QUANTITIES TO THE EIGENSYSTEM

The method described here is applicable to systems which can be described by a linear operator equation, usually an integral equation, of the form

$$\mathcal{L}_s \overline{f} = \overline{g} \tag{1}$$

where s is a complex frequency variable $s = \sigma + j\omega$, $\mathcal{L}_s$ is a linear operator depending on s, $\overline{f}$ is some unknown field quantity, and $\overline{g}$ is the excitation field. For example, a simply connected perfectly conducting scatterer would have an unknown surface current density $\overline{f}$, $\mathcal{L}_s$ would be an integral over the scatterer with a dyadic greens function kernel (depending on s) and $\overline{g}$ would be the incident field.

When the method of moments is used to discretize (1), the following matrix equation results.

$$[M(s)]\,[f] = [g] \tag{2}$$

where $[M(s)]$ is a matrix comprising interactions between bases and testing functions which approximates the operator, $[f]$ is a vector of weights for expansion of $\bar{f}$ in the bases, and $[g]$ is a vector which results from applying the testing functions to $\bar{g}$.

The SEM representation seeks those values of s for which there is a homogeneous solution to (1), and hence to (2). That is,

$$s_n \ni \quad [M(s_n)]\,[f_n] = [0] \tag{3}$$

or within the moment method approximations

$$\mathcal{L}\, s_n \bar{f}_n = 0 \quad . \tag{4}$$

The function $\bar{f}_n$ which obtains from an expansion in terms of $[f_n]$ is termed the *natural mode* corresponding to the *pole* s_n. For all of the perfectly conducting objects of finite extent thus far studied by way of SEM, the poles and natural modes constitute a complete description of the electromagnetic behavior of the object. Typically, planewave coupling coefficients are tabulated as well. They reflect the response of each mode as a function of aspect angle of an

incident plane wave. In practice, it is possible to determine and retain only a finite collection of the poles and associated quantities. This translates into band limitations on the excitation waveforms for which a response can be accurately constructed.

Baum recently presented an interpretation of the SEM representation as described above in terms of classical eigenvalue theory [6]. His interpretation may be summarized, in part, as follows.

Consider the matrix eigenvalue problem associated with (2):

$$[M(s)]\,[f_i(s)] = \lambda_i(s)\,[f_i(s)] \quad . \tag{5}$$

Let s_0 be a pole of (2), i.e., in (3)

$$[M(s_0)]\,[f_0(s_0)] = [0] \quad . \tag{6}$$

It is evident from (6) and (5) that there is a zero eigenvalue in the eigensystem of (5) and that $[f_0]$ is the eigenvector associated with this zero eigenvalue. At issue, of course, is the question, "which eigenvalue of (5) goes to zero?" Baum elaborates on this point in [5] and constructs an ordering scheme associating poles and eigenvalues. It is sufficient for our present purpose to draw two conclusions:

(1) At each pole an eigenvalue of the moment matrix goes to zero.

$$\lambda_0(s) \to 0, \text{ as } s \to s_0$$

(2) This zero eigenvalue is associated with the eigenvector which is identical to the natural mode at the pole.

$$f_0(s) \to f_0, \text{ as } s \to s_0 \quad .$$

In principle, it is possible to use $\lambda_0(s)$ as the objective function of a zero determining scheme. However, in practice, one is forced to rely on numerical schemes for computation of the eigenvalues of [M(s)]. The ordering of the eigenvalues returned from the algorithm will change from one value in s to another so that it is not, in general, possible to track the behavior of a single eigenvalue as a function of s. Also, the computational costs of eigenvalue determination are even greater than that of determinant evaluation.

3. A STATIONARY FORM FOR λ_0

The generalized Rayleigh quotient

$$\lambda_i(s) \overset{1}{=} \frac{[h_i(s)]\,[M(s)]\,[f_i(s)]}{[h_i(s)]^\dagger [f_i(s)]} \tag{7}$$

can be shown to be a stationary form for $\lambda_i(s)$. The vector $[h_i(s)]$

is the biorthogonal vector corresponding to $[f_i(s)]$. That is, it is the eigenvector of $[M(s)]$ associated with $\lambda_i(s)$. (The symbol † denotes transposed conjugate.) In other words the equality in (7) holds to first order. When $[M(s)]$ is Hermitian $[h_i] = [f_i]$ and this expression becomes the familiar Rayleigh quotient. In this case, the eigenvalues are real and the stronger result that (7) is an upper bound to the eigenvalue obtains.

The stationary form (7) may be used to approximate the vanishing eigenvalue provided estimates for $[h_i(s)]$ and $[f_i(s)]$ are available. An observation of the behavior of the moment matrix points to a means for obtaining these estimates.

Let $\mathcal{T}$ denote a triangularization operator constituting Gaussean elimination with maximum element pivoting. Consider the result of this operator applied to $[M(s_0)]$ the moment matrix at a pole location. Namely,

$$[T(s)]\Big|_{s=s_0} = \mathcal{T}[M(s_0)] \quad . \tag{8}$$

This matrix has the following form

$$\begin{bmatrix} t_{11} & t_{12} & \cdots & & t_{1n} \\ 0 & t_{22} & \cdots & & \\ 0 & 0 & & & \\ \vdots & & & & \\ & & 0 & t_{n-1,n-1} & t_{n-1,n} \\ 0 & & 0 & 0 & 0 \end{bmatrix} \tag{9}$$

The determinant of the moment matrix is given by the product of the main diagonal elements of [T].

At a simple pole the moment matrix must have a zero determinant. In the triangularized form (9) the zero of the determinant is manifest as a zero in the lower right position of the matrix. The maximum element pivoting feature of the triangularization operator assures that the zero occurs here. The natural mode $[f_i]$ is determined by prescribing an arbitrary non-zero value for the last element of this vector and "backsolving" the homogeneous matrix equation based on [9] to determine the remaining elements of $[f_i]$.

As a point of interest we might note that since all of the elements in [M(s)] and [T(s)] are analytic in s, in the neighborhood of a simple pole, $t_{nn}(s)$ is linear in $s - s_0$.

A means to obtain estimates for $[f_i]$ and $[h_i]$ results from an observation about $\mathcal{T}[M(s)]$ in the neighborhood of s_0. In this neighborhood, it is observed that the upper triangle of [T(s)] varies slowly in s. Therefore, we may take as an estimate of $[T(s_0)]$, [T(s)] with $t_{nn}(s)$ replaced by zero:

$$[T(s_0)] \approx [T(s)]\Big|_{t_{nn}=0} , \quad s \in N(s_0) . \tag{10}$$

Having this estimate of $[T(s_0)]$ allows us to backsolve the resulting triangular homogeneous system of equations for an estimate to the natural mode. By the same process, we estimate $[h(s_0)]$ from $[M(s)]^\dagger$.

4. AN EFFICIENT COMPUTATIONAL APPROACH TO POLE SEARCHING

The results above can be used to construct a pole-search procedure which is more economical than directly searching for the zeros of the determinant of the moment matrix. The method depends on a reasonable initial estimate for the pole location being sought. This estimate may be determined from physical insight, from tracking the pole trajectory with respect to a geometric parameter, or from Baum's argument number bisection [4, 5] of a region of the left half of the s plane until a pole is localized.

At this first estimate point, the moment matrix is computed. Both the matrix and its tranjugate are triangularized by numerical application of the $\mathcal{T}$ operator. The lower right element in each of the triangularized matrices is set to zero and the resulting homogeneous systems of equations are backsolved for estimates of the natural mode $[f_0]$ and its adjoint companion $[h_0]$. Let us denote these estimates $[f_a]$ and $[h_a]$.

Next, these vectors are used in the variational form (7) with $[M(s)]$ to approximate $\lambda(s)$, viz.,

$$\lambda(s) \approx \frac{[h_a]^\dagger \; [M(s)] \; [f_a]}{[h_a]^\dagger \; [f_a]} \quad . \tag{11}$$

Thus, the eigenvalue at any value of s in a region in the vicinity of a pole may be calculated through one matrix - vector product and two vector - vector products, a total of $N^2 + 2N$ complex "operations." "Operation" is used in the usual sense in the context of matrix computations; that of a multiplication followed by an addition.

The $\lambda(s)$ approximated by (11) is used as the objective function for a complex root locating algorithm such as Muller's method. It is equally applicable to the argument number approach of [4, 5]. The computational economy appears in the form of the reduced number of calculations to derive the search objective function from the moment matrix. The $N^2 + 2N$ operations for the approximation of $\lambda(s)$ pointed out above stands in contrast to the $\frac{1}{3} N^3 + 0(N^2)$ of operations for calculating a determinant. It is both simpler and more economical than direct eigenvalue computation, too. In addition to being costly, eigenvalue computation leaves the problem mentioned above of picking from the eigensystem the eigenvalue which should go to zero in the region of the s plane in question. Because the estimates $[f_a]$ and $[h_a]$ approximate the natural mode and adjoint natural mode for the nearest pole, the appropriate eigenvalue is automatically selected.

We are quick to point out that there is one immediately identifiable liability in the approach suggested here. That is, in taking an

estimate-dependent objective function, we forego any guarantee that convergence in the zero search will converge or that a point converged upon is an actual zero of the matrix. A later example illustrates this feature. It is essential that the method be used only as a companion to either determinant or exact eigenvalue calculations to verify the results obtained. The estimate-dependent feature of the method may be improved upon by periodically updating the estimates $[f_a]$ and $[h_a]$ within the iteration.

In summary, the algorithmic approach is as follows:

(1) At an initial estimate of the pole, calculate the moment matrix for the system. Also form the tranjugate of the moment matrix.

(2) Triangularize these matrices and backsolve them for *estimates* of the eigenvector and its companion biorthogonal vector *at the pole*.

(3) For any s in the vicinity of the pole, the vanishing eigenvalue may be approximated by the generalized Rayleigh quotient

$$\lambda(s) \cong \frac{[h_a]^\dagger\ [M(s)]\ [f_a]}{[h_a]^\dagger\ [f_a]} \quad .$$

(4) Higher accuracy may be obtained in lengthy iterations by periodically performing steps 1 and 2 at a better estimate of the pole as it is obtained through iteration.

5. NUMERICAL RESULTS

As an initial verification of the Rayleigh quotient as an estimator of the eigenvalue, the eigenvalues for a Hallén equation model of a straight wire were computed directly and compared with Rayleigh quotient forms for s values in the vicinity of a pole. The s values used are those along a Muller iteration path which successfully located a zero of the determinant of the moment matrix. The results of this comparison are summarized in Table 1. Rayleigh quotients based on two different eigenvector/biorthogonal vector estimators are given. The "locally-based" value is given by an estimate of the vectors from the moment matrix at the s value for which $\lambda(s)$ is being calculated. The "start-based" value is based on the vector estimates taken at the first s value in the Table.

It is observed that the locally-based eigenvalue approximation tends toward zero in a manner roughly proportional to the determinant. The start-based approximation manifests a thresholding when the s values are coincident with the pole to four significant digits. This phenomenon should be tolerable so long as the zero search algorithm applies a criterion of convergence other than the absolute vanishing of the objective function. For example, the Muller method algorithm which we use terminates upon the magnitude objective function falling below a preassigned error tolerance *or* when the independent variable is invariant to a preassigned number of digits.

TABLE 1

EIGENVALUES AND ESTIMATED EIGENVALUES ALONG A DETERMINANT ZERO SEARCH PATH IN THE MULLER ITERATION: THIN WIRE WITH RADICES/LENGTH = .005

ITERATION PATH (s)	CALCULATED EIGENVALUE	LOCALLY-BASED RAYLEIGH QUOTIENT	START-BASED RAYLEIGH QUOTIENT	CALCULATED DETERMINANT
$-.117 + j1.097^{2}$	$.186 + j.043$	$.186 + j.043$	$.186 + j.043$	$(.328 + j.003)\times10^{5}$
$-.096 + j0.898^{2}$	$(-.279 + j.129)\times10^{-1}$	$(-.279 + j.129)\times10^{-1}$	$(-.290 + j.126)\times10^{-1}$	$(-.425 + j.306)\times10^{4}$
$-.100 + j0.997^{1}$	$(.797 + j.286)\times10^{-1}$	$(.797 + j.286)\times10^{-1}$	$(.788 + j.284)\times10^{-1}$	$(.143 + j.020)\times10^{4}$
$-.083 + j0.923^{3}$	$(-.189 + j.000)\times10^{-3}$	$(-.190 + j.000)\times10^{-3}$	$(-.128 - j.037)\times10^{-2}$	$(-.316 + j.063)\times10^{2}$
$-.083 + j0.923^{4}$	$(-.348 + j.003)\times10^{-6}$	$(-.429 + j.077)\times10^{-6}$	$(-.109 - j.037)\times10^{-2}$	$(-.449 - j.050)\times10^{-1}$
$-.083 + j0.923^{4}$	$(-.373 - j.073)\times10^{-7}$	$(-.2479 + j.1814)\times10^{-6}$	$(-.109 - j.037)\times10^{-2}$	$(.657 - j.086)\times10^{-1}$
$-.083 + j0.923^{4}$	$(-.329 + j.017)\times10^{-7}$	$(-.4431 + j.205)\times10^{-6}$	$(-.109 - j.037)\times10^{-2}$	$(-.418 - j.025)\times10^{-1}$

NOTES ON MULLER ITERATION

1. Starting point given to algorithm - s_i
2. Algorithm generated starting points - $s_i \pm 0.1\ s_i$
3. First prediction for zero
4. Convergence determined by stability to 4 sig. dig. (3 shown)

Table 2 gives the results of pole location determined by Muller's method iteration where the objective function is the start-based Rayleigh quotient. The table also shows the starting of the iteration and the pole values obtained by Tesche [2]. (These data are available in tabular form in [7] also.) The agreement in pole values is seen to be excellent with nominal one percent departures for the first ten poles given. (The first ten are the ten lowest order layer one poles.) The last three values agree to about 2-3 percent. These poles are the three lowest order layer two poles. The "less resonant" inner layer poles are more difficult than the first layer poles to obtain accurately in determinant based schemes, too. It is significant that even the smaller real parts of the poles are accurately determined. The starting points used in this example are the well-known half wavelength resonances of a filamentary dipole for the ten layer one poles.

Figure 1 shows the pole trajectory for the lowest order resonance of a rectangular plate as the aspect ratio w/L is varied. The solid curve was derived by means of Muller iteration on the determinant of the moment matrix for the structure. The dashed line was derived from a start-based Rayleigh quotient. The initial point marked by x was the beginning point for determining the w/L = 1 pole location. The w/L = 1 pole was used as the starting point for the w/L = 0.9 pole. This tracing procedure was continued at w/L decrements of 0.1. The largest error is indicated in the Figure at the w/L = 0.7 pole - an error of 0.47% of the magnitude of the determinant pole.

TABLE 2

COMPARISON OF POLES SEARCHED BY WAY OF GENERALIZED RAYLEIGH QUOTIENT AND THOSE BY WAY OF THE MATRIX DETERMINANT. THIN-WIRE WITH RADIUS/LENGTH = .005

RAYLEIGH QUOTIENT ITERATION		DETERMINANT
STARTING POINT $(\frac{sL}{c\pi})$	DERIVED POLE $(\frac{sL}{c\pi})$	DERIVED POLE $(\frac{sL}{c\pi})$
0.000 + j1.000[1]	-.082 + j0.924	-0.082 + j0.926
0.000 + j2.000[1]	-0.120 + j1.908	-0.120 + j1.897
0.000 + j3.000[1]	-0.146 + j2.900	-0.147 + j2.874
0.000 + j4.000[1]	-0.169 + j3.882	-0.169 + j3.854
0.000 + j5.000[1]	-0.187 + j4.878	-0.188 + j4.835
0.000 + j6.000[1]	-0.204 + j5.864	-0.205 + j5.817
0.000 + j7.000[1]	-0.219 + j6.863	-0.220 + j6.800
0.000 + j8.000[1]	-0.234 + j7.854	-0.234 + j7.783
0.000 + j9.000[1]	-0.247 + j8.847	-0.247 + j8.767
0.000 + j10.000[1]	-0.259 + j9.850	-0.260 + j9.752
-2.000 + j0.000	-2.207 + j.000	-2.174 + j0.0
-2.250 + j1.500	-2.464 + j1.334	-2.506 + j1.347
2.400 + j2.600	-2.707 + j2.346	-2.725 + j2.477

NOTES: 1. Taken as the pole locations of filamentary dipole for first layer poles.

2. From Tesche [2], [6].

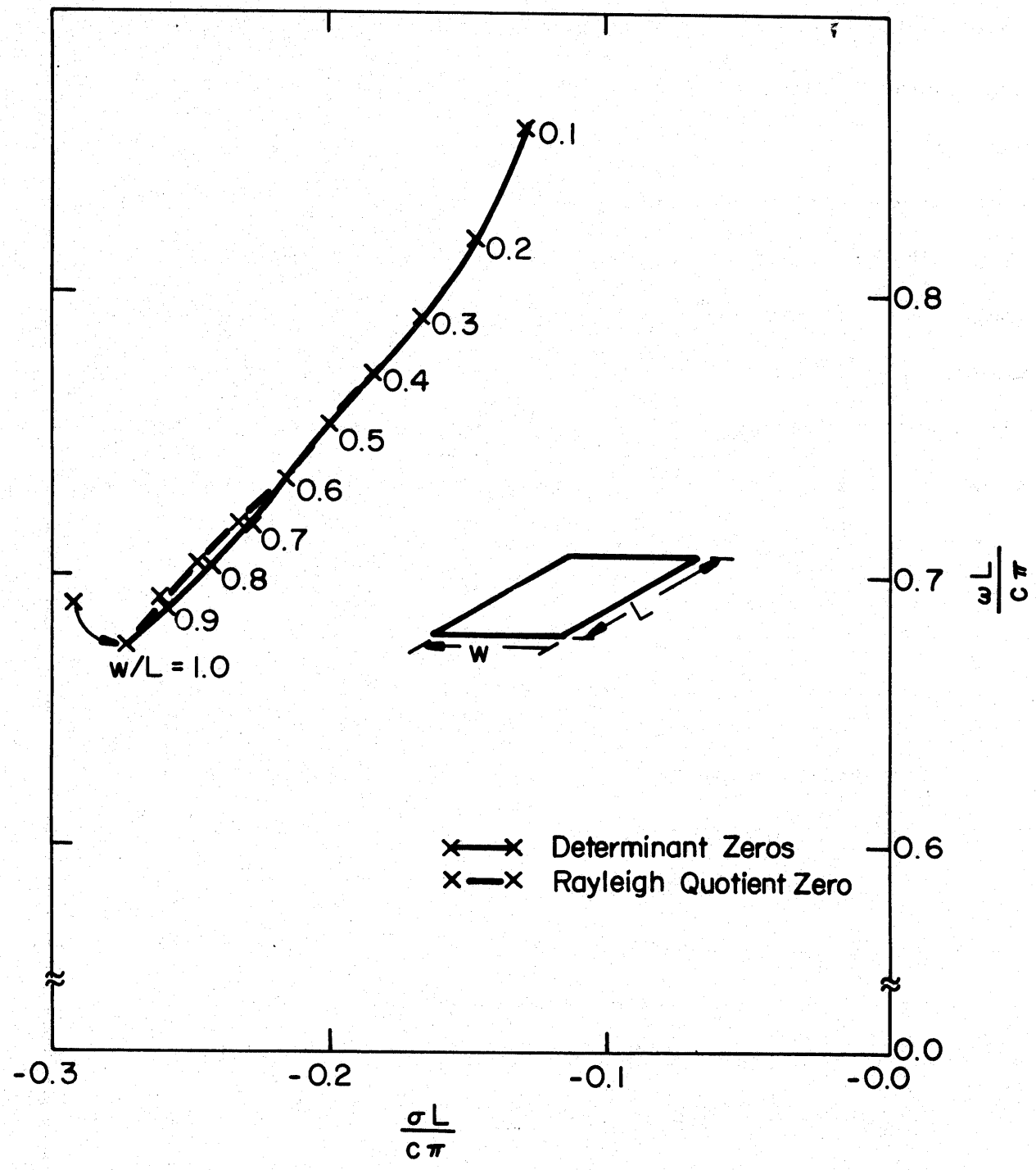

Figure 1. Pole trajectory iteration by way of Rayleigh quotient as compared to the pole trajectory derived from determinant zeros. The structure is a rectangular plate and w/L is under variation.

Figure 2 provides some insight as to the dependence of the pole obtained by the iteration on the starting point of the iteration. The cross indicates the determinant derived pole for the rectangular plate with w/L = 1. The bullet points indicate various starting points for a start-based Rayleigh quotient iteration. Lines connect each starting point with the pole value to which the iteration converged. It is seen that a good estimate of the pole is necessary to get an accurate final estimate of the determinant value. Further, it appears that the direction from the starting estimate to the correct pole influences the outcome of the iteration. This is likely a function of the contours of the determinant value in the region in question.

6. CONCLUSIONS

A method has been developed whereby one may derive a new search objective function for locating SEM poles. This search objective is more economical to calculate than either direct numerical eigenvalues or the determinant of the moment matrix. To the authors' knowledge this work represents the first results which improves the efficiency of computing the search objective itself. Other works such as [4, 5] have dealt with improved use of the determinant objective.

The method is variational in character and rests on the ability to estimate the natural modes of a system. This estimate-dependence introduces some risk into the search for poles. As a result, it is

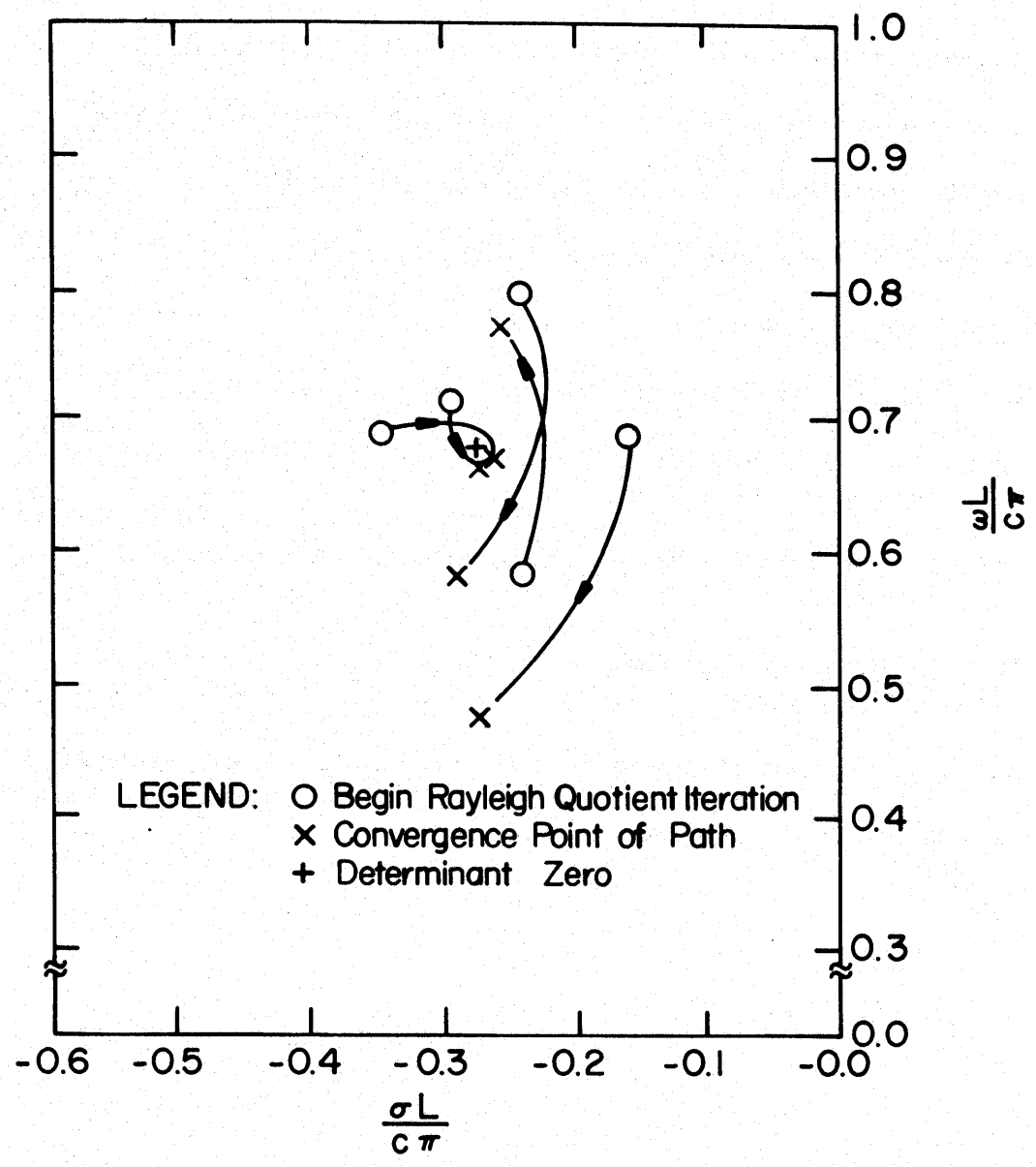

Figure 2. Dependence of the convergence point of the Rayleigh quotient iteration on starting point for the lowest order resonance of a square plate.

likely that poles obtained by the method presented will have to be verified or perhaps refined by means of determinant calculation. The methods potential utility lies in the determination of poles for large bodies where the computation costs are significant. It should be most useful as a companion to determinant-based searches and argument number methods in order to reduce computational costs.

Several methods have the potential for providing a good initial estimate for the pole location:

1. Estimation derived from physical considerations;
2. A crude localizing of the pole based on argument number methods;
3. Trajectory tracing such as that indicated by Figure 2 herein;
4. Utilizing a low-order moment method solution and determinant search.

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