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LETTERS TO THE EDITOR

DISCUSSION ON "NATURE OF STATIONARITY OF THE RAYLEIGH QUOTIENT AT THE NATURAL MODES IN THE RAYLEIGH–RITZ METHOD"

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1. INTRODUCTION

The nature of stationarity of the Rayleigh Quotient was the subject of an article published in 1997 [1]. The major drawbacks of the Rayleigh–Ritz method of finding natural frequencies are the difficulties in obtaining admissible functions and the lack of information on the error bounds [2]. While the use of restraints with very large stiffnesses appears to have alleviated the need to find admissible functions that do not violate any geometric constraint [3–5], this reader is not aware of any general procedure to estimate the maximum possible error in a Rayleigh–Ritz scheme (some method for finding lower bounds are available [6], but these are not easy to apply, generally). For this reason, the article by Prof. Bhat [1] assumes significance because it concludes that the accuracy of natural frequencies computed by energy methods (including the Rayleigh–Ritz method) can be checked by examining whether the computed natural frequencies are minimum at the corresponding computed natural modes. This was demonstrated numerically for some specific systems, but has not been proven to be true for a general case. However it can be shown that the suggested method fails to predict the degree of accuracy for some systems. In fact, as explained in this note, it is not valid even for the systems considered in reference [1] if different functions are chosen as admissible functions. It is possible that the method proposed in reference [1] may apply under certain conditions, but unless such conditions are known, it is unlikely to give reliable prediction of errors or error bounds.

In reference [1], it is stated that in the case of exact natural frequencies and modes, the second derivative of the Rayleigh Quotient given by $K_{jj} - \omega^2 M_{jj}$ is zero, and therefore the frequencies are not stationary with respect to the displacement coefficients Q_j. However, it is well established that each of the frequencies calculated using the Rayleigh–Ritz method is indeed a minimum [6–8]. Furthermore, since the Rayleigh–Ritz modes are also orthogonal to each other (in the limited Rayleigh–Ritz manifold) it is possible to express the eigenvalue equations in a decoupled form (as for the exact modes) resulting in zero values for K_{jj}—$\omega^2 M_{jj}$. This may be demonstrated by studying the cantilever problem treated in reference [1].

2. RAYLEIGH–RITZ ANALYSIS OF A CANTILEVER BEAM

Expressing the displacement $X(x)$ in terms of admissible functions,

$$X(x) = \sum_{i=1}^{4} Q_i f_i(x), \tag{1}$$

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where the admissible functions used in reference [1] are

$$f_1(x) = x^2; \; f_2(x) = x^3; \; f_3(x) = x^4; \; f_4(x) = x^5. \qquad (2a, b, c, d)$$

Let us use the calculated modes from a Rayleigh–Ritz analysis using the above set of functions as admissible functions. This gives

$$f_1(x) = 0{\cdot}913x^2 - 0{\cdot}4x^3 - 0{\cdot}052x^4 + 0{\cdot}059x^5, \qquad (3a)$$

$$f_2(x) = 0{\cdot}373x^2 - 0{\cdot}797x^3 + 0{\cdot}469x^4 - 0{\cdot}074x^5, \qquad (3b)$$

$$f_3(x) = -0{\cdot}154x^2 + 0{\cdot}602x^3 - 0{\cdot}732x^4 + 0{\cdot}279x^5, \qquad (3c)$$

$$f_4(x) = -0{\cdot}097x^2 + 0{\cdot}492x^3 - 0{\cdot}775x^4 + 0{\cdot}384x^5. \qquad (3d)$$

This would result in diagonal stiffness and mass matrices and at the calculated frequencies

$$\partial^2\omega^2/\partial Q_j^2 = K_{jj} - \omega^2 M_{jj} = 0. \qquad (4)$$

(The notation used here is the same as that in reference [1].) The frequency parameters calculated would be the same as in reference [1] (3·516, 22·158, 63·347, 281·596). The frequencies for the first two modes agree well with exact results (exact values being 3·5156, 22·034, 61·6972, 120·9019) but for the third mode, there is a noticeable deviation and there is no agreement for the fourth one. The fact that the fourth frequency deviates substantially from the exact value while the first two are in good agreement, cannot be discovered by checking the sign of $\partial^2\omega^2/\partial Q_j^2$.

2.1. ANALYSIS WITH TWO SPECIFIC ADMISSIBLE FUNCTIONS

Now let us consider the results with the following two-term Rayleigh–Ritz solution: Using

$$X(x) = \sum_{i=1}^{2} Q_i f_i(x), \qquad (5)$$

where

$$f_1(x) = 4x^2 - 8x^3 + 5x^4 \;\text{ and }\; f_2(x) = x^2 - 4x^3 + 5x^4 \qquad (6a, b)$$

gives the stiffness and mass matrices as follows:

$$[K] = \begin{bmatrix} 48EI/L^3 & 96EI/L^3 \\ 96EI/L^3 & 228EI/L^3 \end{bmatrix} \;\text{ and }\; [M] = \begin{bmatrix} 53mL/315 & 139mL/630 \\ 139mL/630^3 & 113mL/315 \end{bmatrix}. \qquad (7a, b)$$

Solving $[K] = \omega^2[M]$ with these matrices, we arrive at the following non-dimensional frequency parameters (given by $\omega L^2\sqrt{m/EI}$) and modes:

$$\text{non-dimensional frequency parameters}: \begin{Bmatrix} 12{\cdot}423 \\ 33{\cdot}469 \end{Bmatrix} \qquad (8a)$$

$$\text{mode 1}: \; \{Q\}^{(1)} = \begin{Bmatrix} 1 \\ -0{\cdot}356 \end{Bmatrix} \;\text{ and mode 2}: \; \{Q\}^{(2)} = \begin{Bmatrix} 1 \\ 0{\cdot}929 \end{Bmatrix}. \qquad (8b, c)$$

Comparing these with the exact results, we find that the deviation between the Rayleigh–Ritz and exact values for the first and second frequencies are 254 and 52% respectively.

The second derivatives of the Rayleigh Quotient $\partial^2\omega^2/\partial Q_j^2$ at the calculated frequencies are as follows:

$\partial^2\omega^2/\partial Q_1^2 = 22{\cdot}03$ (positive) at the first calculated frequency and $-140{\cdot}5$ (negative) at the second frequency.

$\partial^2\omega^2/\partial Q_2^2 = 172{\cdot}6$ (positive) at the first calculated frequency and $-173{\cdot}8$ (negative) at the second frequency.

The above figures clearly show that the sign of the second derivative cannot generally be taken as an indicator of the accuracy of a Rayleigh–Ritz solution.

Another point worth considering here is that the type of stationarity of the calculated frequencies in a Rayleigh–Ritz procedure has been shown to be minimum but one needs to bear in mind that this is subject to the orthogonality conditions. That is, with the exception of the highest natural frequency in a finite degree of freedom system, the calculated value of the rth frequency would be a minimum (and upperbound to that of the exact frequency) in the Rayleigh–Ritz manifold subject to $(r-1)$ orthogonality conditions [6, 8]. This may be demonstrated by applying the orthogonality constraints to the lower modes and investigating the variation of the Rayleigh Quotient near the calculated frequencies as follows.

2.2. ANALYSIS WITH FOUR SIMPLE POLYNOMIALS AS ADMISSIBLE FUNCTIONS

Let us now revisit the solution developed in reference [1], with admissible functions given by equation (2a–c) but this time applying the conditions that the higher modes are orthogonal to the previous modes. Let us consider the third mode as an example. The statements of orthogonality of the third mode with respect to the first two modes may be written as

$$\int_0^L m(Q_1x^2 + Q_2x^3 + Q_3x^4 + Q_4x^5)(0{\cdot}913x^2 - 0{\cdot}4x^3 - 0{\cdot}052x^4 + 0{\cdot}059x^5)\,\mathrm{d}x = 0, \qquad (9a)$$

$$\int_0^L m(Q_1x^2 + Q_2x^3 + Q_3x^4 + Q_4x^5)(0{\cdot}373x^2 - 0{\cdot}797x^3 + 0{\cdot}469x^4 - 0{\cdot}074x^5)\,\mathrm{d}x = 0. \qquad (9b)$$

The mass per unit length, m and length, L for the beam may be taken as unity, since only non-dimensional parameters are required. On substitution and integration, equations (9a) and (9b) reduce to

$$0{\cdot}115880\,Q_1 + 0{\cdot}095080\,Q_2 + 0{\cdot}080551\,Q_3 + 0{\cdot}069844\,Q_4 = 0, \qquad (9c)$$

$$-0{\cdot}000483\,Q_1 - 0{\cdot}001288\,Q_2 - 0{\cdot}001628\,Q_3 - 0{\cdot}001758\,Q_4 = 0. \qquad (9d)$$

From these two equations, we can arrive at the following relationships between various Q_i values:

$$Q_3 = -6{\cdot}096\,Q_1 - 2{\cdot}769\,Q_2, \quad Q_4 = 5{\cdot}3716\,Q_1 + 1{\cdot}8324\,Q_2. \qquad (10a,b)$$

To consider the variation of the Rayleigh Quotient in the neighbourhood of the third mode, it is important to adjust the coefficients Q_3 and Q_4 to allow for equations (10a,b) to be satisfied. With these constraints, we may plot the variation of the frequency parameter ω^2 (the Rayleigh Quotient) in the neighbourhood of the third calculated frequency parameter of 63·347. The variation of ω^2 with Q_1 for $Q_2 = 0{\cdot}602$ and with Q_2 for $Q_1 = -0{\cdot}154$ are shown in Figures 1 and 2. These plots clearly show that the Rayleigh Quotient is a minimum in the neighbourhood of the third calculated natural frequency. The difference between these figures and Figures 1(i) and 1(j) in reference [1] is that the present figures are based on Rayleigh Quotients calculated after applying the constraint conditions. Similarly the variation of the Rayleigh Quotient with Q_3 or Q_4 can be obtained by expressing Q_1 and Q_2 in terms of Q_3 and Q_4 using equations (9c,d). This would confirm that the Rayleigh Quotient is a minimum at the third calculated frequency with respect to

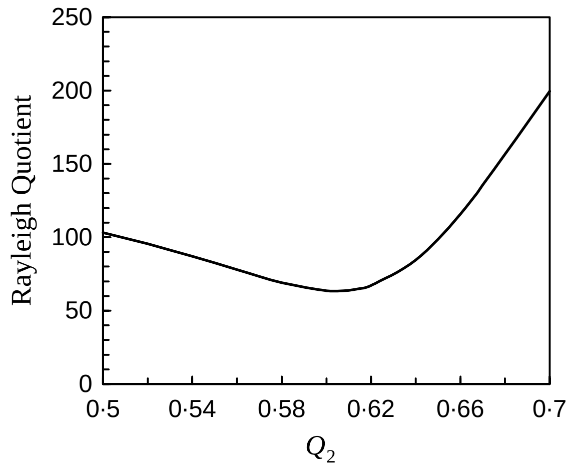

Figure 1. Variation of the Rayleigh Quotient with Q_2, for $Q_1 = -0{\cdot}154$.

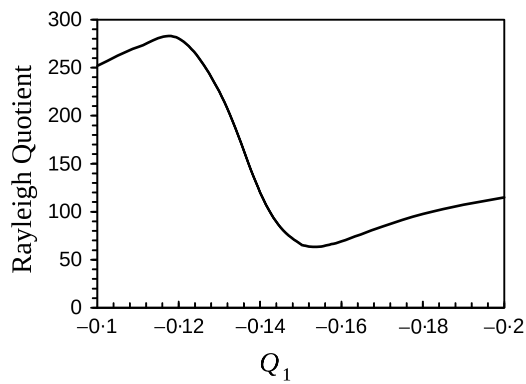

Figure 2. Variation of the Rayleigh Quotient with Q_1, for $Q_2 = 0{\cdot}602$.

Q_3 and Q_4 also. (The difference between the stationarity of the Rayleigh Quotient at higher modes with and without the application of the constraint condition is analogous to finding the minimum of a surface and the minimum of the surface in a plane that is defined by an orthogonality condition.)

Another way to demonstrate the nature of stationarity of the calculated frequencies is to use the Lagrangian multiplier method. This would require modification of the stiffness matrix in reference [1] which would now include the constraint conditions associated with Lagrangian multipliers. To illustrate this, let us apply the orthogonality conditions given by equations (9c) and (9d) as the Lagrangian constraints. This gives the following modified matrices:

$$[K] = \begin{bmatrix} 4 & 6 & 8 & 10 & 0{\cdot}115880 & -0{\cdot}000483 \\ 6 & 12 & 18 & 24 & 0{\cdot}095080 & -0{\cdot}001288 \\ 8 & 18 & 28.8 & 40 & 0{\cdot}080551 & -0{\cdot}001628 \\ 10 & 24 & 40 & 400/7 & 0{\cdot}069844 & -0{\cdot}001758 \\ 0{\cdot}115880 & 0{\cdot}095080 & 0{\cdot}080551 & 0{\cdot}069844 & 0 & 0 \\ -0{\cdot}000483 & -0{\cdot}001288 & -0{\cdot}001628 & -0{\cdot}001758 & 0 & 0 \end{bmatrix} \tag{11a}$$

$$\text{and } [M] = \begin{bmatrix} 1/5 & 1/6 & 1/7 & 1/8 & 0 & 0 \\ 1/6 & 1/7 & 1/8 & 1/9 & 0 & 0 \\ 1/7 & 1/8 & 1/9 & 1/10 & 0 & 0 \\ 1/8 & 1/9 & 1/10 & 1/11 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{11b}$$

Solving $[K] = \omega^2[M]$ with the above matrices would give only two natural frequencies which are 63·347 and 281·596. The lowest for this system is the third calculated mode for the original problem, but now with the constraint condition, it is the lowest (globally) within the constrained domain of admissible functions.

In reference [1], the variation of the calculated natural frequency against the frequencies corresponding to selected admissible functions was also investigated. Once again, if conditions of orthogonality with respect to lower modes are applied, these procedures would also result in minimum values for the frequencies.

3. CONCLUDING REMARKS

The results presented here show that the sign of the second derivative of the Rayleigh Quotient is not necessarily a good indicator of the degree of accuracy of the frequencies calculated using a Rayleigh–Ritz procedure, and illustrate the nature of stationarity of the frequencies. As expected, the Rayleigh Quotient, and hence the frequency estimates, are minimum in the neighbourhood of the calculated modes, if conditions of orthogonality of the higher modes with all the lower modes are enforced.

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