Successive Approximations by the Rayleigh-Ritz Variation Method

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Approximate eigenvalues given by the Rayleigh-Ritz variation method for handling linear differential equations are examined and relations are established between the discrete eigenvalues obtained in successive approximations. These relations should be of use in practical computations. A method for fixing upper bounds to eigenvalues is given and a procedure previously employed by the writer to simplify determinant calculations is adapted for use in the present theory.

THE variation method[1] of Rayleigh and Ritz has found frequent application in the determination of approximate solutions for differential equations arising in physical problems. Considerations of "eits" and "eifs" (Bateman's[2] useful abbreviations for "Eigenwerte" and "Eigenfunktionen") for excited wave mechanical systems have indicated that there are points which require study. This note is a result of such investigation. Certain aspects of the behavior of eits in successive approximations are examined here but no attempt is made to consider convergence or approximate eits for continuous ranges.

For definiteness our equations are summarized. A linear differential equation[3] in variables $x_1, x_2, \cdots, x_N$ is considered:

$$[H(x_1, \cdots, x_N, \partial/\partial x_1, \cdots, \partial/\partial x_N) - W_c]\Psi_c(x_1, \cdots, x_N) = 0 \equiv [H - W_c]\Psi_c = 0. \tag{1}$$

W_c is a correct eit associated with a correct eif Ψ_c. Corresponding approximations W_a and Ψ_a are given by the following equations:

$$\Psi_a = \sum_{n=1}^{m} c_n \Phi_n(x_1, \cdots, x_N), \tag{2}$$

$$\int \Psi_a^* \Psi_a d\tau = 1, \qquad \delta \int \Psi_a^* H \Psi_a d\tau = 0, \qquad \int \Psi_a^* H \Psi_a d\tau = W_a. \tag{3}$$

In these equations $\Phi_1, \cdots, \Phi_m$ are m linearly independent known functions which satisfy the boundary conditions.[3] The δ refers to a first variation applied to the c_n's. The volume element of the $x_1, \cdots, x_N$-space is $d\tau$. The assumed properties of H and of the Φ's give

$$H_{ij}\left(= \int \Phi_i^* H \Phi_j d\tau\right) = H_{ji}^*; \qquad \text{we shall use} \qquad \delta_{ij} = \int \Phi_i^* \Phi_j d\tau = \delta_{ji}^*.[4] \tag{4}$$

Eqs. (2), (3) and (4) give

[1] See: N. Kryloff, Mem. des Sci. Math. fasc. XLIX (1931); also, K. Hohenemser, *Die Methoden zur Angenaherten Losung von Eigenwertproblemen in der Elastokinetic*, pp. 27–30, Berlin, Springer, (1932); also, Kemble, Rev. Mod. Phys. **1**, 206 (1929).

[2] Bateman, *Partial Differential Equations of Mathematical Physics*, preface, Cambridge (1932).

[3] Self-adjointness is assumed together with quadratic integrability of the solutions concerned, and the vanishing of the "bilinear concommitant" on the boundary. See: E. L. Ince, *Ordinary Differential Equations*, p. 123, Longmans (1927); also H. Weyl, Math. Ann. **68**, 220 (1910).

[4] This $\delta_{ij} = \delta(i, j) = \begin{matrix} 0 \\ 1 \end{matrix} \begin{matrix} i \neq j \\ i = j \end{matrix}$ if the Φ's form a normalized orthogonal set, otherwise $\delta_{ij} \neq \delta(i, j)$.

$$\int \Phi_i^*(H-W_a)\Psi_a d\tau = 0 = \sum_{j=1}^{m}(H_{ij}-W_a\delta_{ij})c_j, \quad i=1, 2, \cdots, m; \qquad \sum_{i=1}^{m}\sum_{j=1}^{m} c_i^*\delta_{ij}c_j = 1, \tag{5}$$

whence the m-rowed determinant

$$D_m(W_a) = \left(H_{ij}-W_a\delta_{ij}\right) = 0 \tag{6}$$

From (6) we may obtain the m real roots[5] $W_a = W_{m1}, W_{m2}, \cdots, W_{mm}$ with corresponding $\Psi_a = \Psi_{m1}, \Psi_{m2}, \cdots, \Psi_{mm}$. For the latter, $\Psi_{mk} = \sum_{n=1}^{m} c_{mk,n}\Phi_n$ where the c's are determined by (5) with $W_a = W_{mk}$.

It should be noted that the approximations $\Psi_{m1}, \cdots, \Psi_{mm}$, like the correct Ψ_a's, form an orthogonal set. This orthogonality follows from (4) and (5) thus:

$$\int [\Psi_{mi}^*(H-W_{mj})\Psi_{mj} - \Psi_{mj}(H-W_{mi})^*\Psi_{mi}^*]d\tau = 0 = (W_{mi}-W_{mj})\int \Psi_{mi}^*\Psi_{mj}d\tau$$

$$\therefore \quad \int \Psi_{mi}^*\Psi_{mj}d\tau = \delta(i,j) \quad i,j=1, 2, \cdots, m.^{6} \tag{7}$$

The "next approximation" in which is included another independent function Φ_{m+1} will be considered now. For convenience $\Psi_{m1}, \cdots, \Psi_{mm}$ and Φ_{m+1} will be used as our independent functions. Φ_{m+1} is formed by the usual processes[7] to be normalized and orthogonal to $\Phi_1, \cdots, \Phi_m$. The new determinant analogous to (6) is

$$D_{m+1}(W_a) = \begin{vmatrix} W_{m1}-W_a, & 0, & \cdots, & 0, & h_1 \\ 0, & W_{m2}-W_a, & \cdots, & 0, & h_2 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0, & 0, & \cdots, & W_{mm}-W_a, & h_m \\ h_1^*, & h_2^*, & \cdots, & h_m^*, & h_{m+1}-W_a \end{vmatrix} = G_{m+1}(W_a) - F_{m-1}(W_a) = 0. \tag{8}$$

In (8)

$$h_r = \int \Psi_{mr}^* H\Phi_{m+1}d\tau, \quad r=1, 2, \cdots, m; \qquad h_{m+1} = \int \Phi_{m+1}^* H\Phi_{m+1}d\tau;$$

$$G_{m+1}(W_a) = (h_{m+1}-W_a)\prod_{k=1}^{m}(W_{mk}-W_a); \qquad F_{m-1}(W_a) = \sum_{r=1}^{m}|h_r|^2 \prod_{k,\,k\neq r}^{m}(W_{mk}-W_a).$$

It is convenient to name the eits in increasing sequence thus: $W_a \equiv W_{m1} \leq W_{m2} \leq \cdots \leq W_{mm}$ for the "m-th approximation" eits pertaining to (6); also $W_a \equiv W_{m+1\,1} \leq W_{m+1\,2} \leq \cdots \leq W_{m+1\,m+1}$ for the "$(m+1)$-th approximation" eits pertaining to (8). To determine qualitatively the positions of the $(m+1)$-th relative to the m-th approximation eits consider the following:

$$D_{m+1}(W_{mr}) = -|h_r|^2 \prod_{k,\,k\neq r}^{m}(W_{mk}-W_{mr}) \quad \begin{matrix} \geq 0 \text{ if } r \text{ even}, \\ \leq 0 \text{ if } r \text{ odd} \end{matrix} \quad \text{since } (W_{mk}-W_{mr}) \quad \begin{matrix} \leq 0 \text{ if } k<r. \\ \geq 0 \text{ if } k>r. \end{matrix}$$

[5] Courant and Hilbert, *Mathematische Physik I*, p. 24, Springer (1931). See also Note (8).

[6] Strictly speaking suitable linear combinations of approximate eifs in a degenerate set must be made in order to have (7) hold within such a set.

[7] Whittaker and Watson, *Modern Analysis*, p. 224, Cambridge (1920). This procedure is, of course, only one of convenience and it will not affect the final results.

Also

$$D_{m+1}(W_a)\to\infty \quad \text{as} \quad W_a\to-\infty \quad \text{and} \quad D_{m+1}(W_a)\to(-)^{m+1}\infty \quad \text{as} \quad W_a\to\infty.$$

Therefore $D_{m+1}(W_a)$ must have at least one root between each succeeding two of the following W_a-values: $-\infty$, W_{m1}, W_{m2}, $\cdots$, W_{mm}, ∞. That there is *only one* root between each two follows from the fact that $D_{m+1}(W_a)$ can have only $m+1$ roots. Thus there is the rule:

(*1*) The m-th approximation eits separate those of the $(m+1)$-th approximation, i.e.,

$$W_{m+1\ 1}\leq W_{m1}\leq W_{m+2\ 2}\leq\cdots\leq W_{m+1\ m}\leq W_{mm}\leq W_{m+1\ m+1}.^{8}$$

Corollary 1.1 The p-th lowest eit, W_{mp}, of the m-th approximation is greater than (or equal to) the p-th lowest eit of any succeeding approximation, and therefore, assuming convergence of the process,[9] greater than (or equal to) the p-th lowest correct eit W_{cp}, i.e., $W_{mp}\geq W_{m+q\ p}\geq W_{cp}$ $q>0$.

It is "natural" to consider $W_{m+1\,1}$, $\cdots$, $W_{m+1\ s}$, $W_{m+1\ s+1}$, $W_{m+1\ s+2}$, $\cdots$, $W_{m+1\ m+1}$ as corresponding to[10] (or arising from) W_{m1}, $\cdots$, W_{ms}, h_{m+1}, $W_{m\ s+1}$, $\cdots$, W_{mm} respectively where h_{m+1} is greater than W_{ms} and (or)[11] less than $W_{m\ s+1}$. Then there is:

Corollary 1.2 Any m-th approximation eit which is {less/greater} than h_{m+1} $(=\int\Phi_{m+1}{}^{*}H\Phi_{m+1}d\tau$, Φ_{m+1} normalized and orthogonal to Φ_1, Φ_2, $\cdots$, $\Phi_m)$ is {greater/less} than its corresponding $(m+1)$-th approximation eit, i.e., $W_{m+1\ r}\leq W_{mr}$ $r\leq s$ and $W_{m+1\ r+1}\geq W_{mr}$ $r>s$. h_{m+1} "repels" eits.

(*2*) The eit $W_{m+1\ s+1}$ corresponding to h_{m+1} is such that $W_{m+1\ s+1}\overset{\geq}{\leq}h_{m+1}$ if

$$(-)^{s}D_{m+1}(h_{m+1})\left[=\left(\sum_{r=1}^{s}-\sum_{r=s+1}^{m}\right)|h_r|^2\prod_{\substack{1\\ k,\ k\neq r}}^{m}|(W_{mk}-h_{m+1})|\right]_{\leq 0}^{\geq 0}$$

since $(-)^{s}D_{m+1}(W_{ms})\geq 0\geq(-)^{s}D_{m+1}(W_{m\ s+1})$ and since $D_{m+1}(W_a)$ can have but one root between W_{ms} and $W_{m\ s+1}$.

Corollary 2.1 If $h_{m+1}\leq W_{m1}$ then $W_{m+1\ 1}\leq h_{m+1}$; or if $h_{m+1}\geq W_{mm}$ then $W_{m+1\ m+1}\geq h_{m+1}$.
Corollary 2.2 If $W_{mr}=W_{mr+1}$, $r=1, 2, \cdots$ or $m-1$ then $W_{m+1\ s}=h_{m+1}$.

Corollary 1.1 is perhaps the most important one from a practical viewpoint; to avoid its misuse the following must be realized clearly. If it is desired to fix an upper bound to the p-th lowest correct eit it is *sufficient* to use *at least* p independent functions in the variation process. This condition may be regarded as *necessary* when there is no *a priori* knowledge of the correct eifs—the usual situation in practice. For example, if a single normalized function Φ were used to determine an approximate eit $W_a=\int\Phi^{*}H\Phi d\tau$, then it would not *necessarily* follow that $W_a\geq W_{c2}$, although, of course, $W_a\geq W_{c1}$ would hold true. It is also not necessarily true that if $W_a=W_{cn}$,

[8] The writer wishes to thank Professor H. Bateman of Pasadena for drawing his attention to the fact that this theorem is equivalent to one already known in algebraic theory. The following references are relevant: Hermite, Comptes Rendus, **41** and "Ouvres," **1**, 479; Salmon, *Higher Algebra*, section 47; Burnside and Panton, *Theory of Equations*, Vol. 2, p. 65; C. W. Borchardt, J. de Math. (1) **12**, 50–67 (1847); a slightly more general theorem is given by Bateman, Bull. Am. Math. Soc. **18**, 179 (1912).

[9] Formally the difficulty of continuous ranges of eits may be avoided in the treatment of an eif associated with a discrete eit as follows: assume that the Φ's are chosen so that they ultimately form a complete enough set to give correct expansions for a smaller set (of say, t members) of discrete, correct eifs. The Φ's will all be of the discrete type and some of them may be formed by integration over a range of their "eits." However it must be noted that of the eits determined finally by the use of these Φ's only t of them will be necessarily correct.

[10] Of course in such discontinuous operations as are used here correspondences are necessarily arbitrary. In a sense each approximate eit contains elements of all the correct eits.

[11] The "or" refers to the case $h_{m+1}>W_{mm}$ or $h_{m+1}<W_{m1}$. The possibility of $h_{m+1}=W_{ms}$ or $W_{m\ s+1}$ is not excluded.

$n>1$, then $\Psi_a=\Psi_{cn}$.[12] The necessity of using at least p functions to fix an upper bound for the p-th eit will lead often to determinants of five or more rows and columns. For such many-rowed determinants the calculation of the roots may be prohibitively long in actual cases unless simplified by determinant manipulation. A many-rowed form like Eq. (6) can be replaced by any one of a variety of few-rowed determinants and, in this way, the calculations for certain roots will probably be shortened. For example, a small group of μ members in our set $\Phi_1, \Phi_2, \cdots, \Phi_m$ may be "physically important" for a certain group of eits, which means usually that non-diagonal terms may be small compared with diagonal terms in the part of the m-rowed determinant bordering the μ-rowed "underdeterminant." The contributions of these terms for the eits concerned may be calculated by means of an adaptation of the perturbation method used in a previous paper by the writer.[13] Other methods may be suggested by the forms of particular determinants.

[12] This fact introduces the question of what is meant by "best approximation." If an approximate eit is defined by $W_a=\int\Psi_a^*H\Psi_a d\tau$, $\Psi_a=\Sigma_1^m c_n\Phi_n$ it is always possible (at least in theory) to choose c's and Φ's such that $W_a=W_{cn}$ although a variation process might not lead to a similar result for a given set of fundamental Φ's. The term "best approximation" must refer in the final analysis to the use to which the W_a and the Ψ_a will be put.

[13] J. K. L. MacDonald, Proc. Roy Soc. (London) **A138**, 187 (1932). For present use the reference's Eqs. (9) and (10) are replaced by our (2), (3) and (5). $\Sigma_{s=1}^{\mu}(H_{rs}+\epsilon_{rs}-W_a\delta_{rs})c_s=0$ $r=1, 2, \cdots, \mu$ is substituted for Eq. (15). $(H_{r\sigma}-W_a\delta_{r\sigma})$ and $(W_a\delta_{\sigma s}-H_{\sigma s})/(H_{\sigma\sigma}-W_a\delta_{\sigma\sigma})$ replace $W_{r\sigma}$ and $\Omega_{\sigma s}$ in Eq. (16) of the reference, and σ ranges from $\mu+1$ to m.