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VARIATIONAL PROCEDURE AND GENERALIZED LANCZOS RECURSION FOR SMALL-AMPLITUDE CLASSICAL OSCILLATIONS

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Variational procedure is developed that yields lowest frequencies of small-amplitude oscillations of classical Hamiltonian systems. Genuine Lanczos recursion is generalized to treat related non-Hermitian eigenvalue problems.

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Normal modes ξ and frequencies ω of small oscillations of a classical system near the equilibrium are determined by the secular equation [1]

$$\omega^2 M\xi = K\xi, \tag{1}$$

where M and K are $N \times N$ symmetric positive definite matrices of mass coefficients and spring constants respectively. In many applications the number N of degrees of freedom is large, while only a few lowest frequencies are of interest [2]. Equation (1) represents a problem more complex than a regular symmetric eigenvalue problem, unless M or K is diagonal.

Eq.(1) can be transformed into the Hamiltonian form by introducing canonical momentum $\eta = \omega M\xi$:

$$K\xi = \omega\eta, \qquad T\eta = \omega\xi, \tag{2}$$

where $T = M^{-1}$. Thus, the frequencies of the normal modes are the eigenvalues of a $2N \times 2N$ matrix

$$\begin{pmatrix} 0 & T \\ K & 0 \end{pmatrix}. \tag{3}$$

The spectrum of this matrix consists of pairs $\pm\omega$, since $(\xi, -\eta)$ is also a solution of (2) that corresponds to $-\omega$. The lowest frequency ω_{min} is the lowest *positive* eigenvalue of the matrix (3).

Although the eigenvalues of the matrix (3) are always real, the matrix itself is non-Hermitian, unless $K = T$. Therefore, its diagonalization poses a formidable task. The major problem is that no general minimum principle exists that yields eigenvalues of arbitrary diagonalizable non-Hermitian matrices. This does not allow to formulate a variational procedure similar to the Rayleigh-Ritz procedure for Hermitian matrices. If $K = T$, the matrix (3) is Hermitian, and its positive eigenvalues coincide with those of K and T.

As known from quantum mechanics, the lowest eigenvalue ϵ_{min} of a Hermitian matrix H can be obtained from the minimum principle

$$\epsilon_{min} = \min_{\{\psi\}} \frac{(\psi H\psi)}{(\psi\psi)}. \tag{4}$$

The minimum is to be searched over all vectors ψ. The Ritz variational procedure is an approximation when the set $\{\psi\}$ in (4) is restricted to some subspace $\mathcal{K}$ of dimension $n < N$. The best approximation to ϵ_{min} in the sense of (4) is obtained as the lowest eigenvalue of the $n \times n$ Rayleigh matrix $\widetilde{H}$, obtained by projection of H onto $\mathcal{K}$.

The special paired structure of the matrix (3) makes it possible to generalize (4) such as to yield ω_{min}. In fact,

$$\omega_{min} = \min_{\{\xi,\eta\}} \frac{(\xi K \xi) + (\eta T \eta)}{2\,|(\xi\eta)|}. \tag{5}$$

The minimum is to be searched over all possible phase space configurations $\{\xi, \eta\}$. Before providing the proof to this equation let me point out some of its features.

First, it states that ω_{min} is the minimum arithmetic mean of $(\xi K \xi)$ and $(\eta T \eta)$ over all pairs of vectors ξ, η with scalar product $(\xi\eta) = 1$. Since K and T are both positive definite, the right-hand side is strictly positive and so is ω_{min}. Second, eq.(5) is symmetric in K and T, according to the nature of the problem. When $K = T$ the minimum is achieved at $\xi = \eta$, and (5) becomes the same as (4).

Note that the functional in (5) has no maximum, since the denominator can be made arbitrarily small. The global minimum, however, always exists. This is not obvious, since a set of all pairs of vectors with $(\xi\eta) = 1$ is not compact. Indeed, say, any vector orthogonal to η can be added to ξ, making $|\xi|$ arbitrarily large. However, the functional in (5) grows indefinitely in this case, such that the global minimum is achieved at finite $|\xi|$ and $|\eta|$.

Variation of (5) with respect to ξ and η yields eq.(2). Thus, the solutions of (2) are the stationary points of (5). The global minimum (5), therefore, gives indeed ω_{min}. The singularity in the denominator poses no problem, since it corresponds to infinitely large values of functional, while near the minimum it is analytic.

Minimum principle (5) can, in fact, be obtained from the Thouless minimum principle [3], derived for non-Hermitian matrices that appear in random phase approximation (RPA). Eq.(5) transforms into the Thouless minimum principle by substitution: $A = (K + T)/2$, $B = (K - T)/2$, $x = (\xi + \eta)/2$, and $y = (\xi - \eta)/2$.

Variational procedure similar to the Rayleigh-Ritz procedure can be formulated if coordinates ξ and momenta η in (5) are restricted to some subspaces $\mathcal{U}$ and $\mathcal{V}$ of dimension n, respectively.

Let $\{\xi_i\}$ and $\{\eta_i\}$ be two sets of vectors that span $\mathcal{U}$ and $\mathcal{V}$, such that $(\xi_i\eta_j) = \delta_{ij}$. Expanding $\xi = \sum u_i\xi_i$, $\eta = \sum v_i\eta_i$ and varying (5) with respect to u_i and v_i, we find the latter to obey a $2n \times 2n$ eigenvalue equation

$$\begin{pmatrix} 0 & \widetilde{T} \\ \widetilde{K} & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \widetilde{\omega} \begin{pmatrix} u \\ v \end{pmatrix}, \tag{6}$$

with $\widetilde{K}_{ij} = (\xi_i K \xi_j)$ and $\widetilde{T}_{ij} = (\eta_i T \eta_j)$. Eq.(6) generalizes Hermitian Rayleigh-Ritz eigenvalue equation for $\widetilde{H}$. It has $2n$ solutions $\pm\widetilde{\omega}$, the lowest positive of which gives the best approximation to ω_{min} in the sense of eq.(5).

Krylov subspace [2] for the matrix (3) can be constructed by acting with it many times on an arbitrary vector (ξ_1, η_1):

$$\begin{pmatrix} \xi_1 \\ \eta_1 \end{pmatrix}, \begin{pmatrix} T\eta_1 \\ K\xi_1 \end{pmatrix}, \begin{pmatrix} TK\xi_1 \\ KT\eta_1 \end{pmatrix}, \cdots \tag{7}$$

The subspace that spans first n vectors of this sequence has the property of approximating an invariant subspace of (3). Thus, it is natural to expand approximation to an eigenvector of (3) as a linear combination of these vectors. In other words, the natural choice for the subspaces $\mathcal{U}$ and $\mathcal{V}$ for the variational procedure described above are the subspaces $\mathcal{U}_n$ and $\mathcal{V}_n$ that span the upper and lower components of first n vectors of (7).

In order to implement the variational procedure, it is necessary to construct a biorthogonal basis $\{\xi_i, \eta_i\}$, $i = 1, ..., n$ in $\mathcal{U}_n$ and $\mathcal{V}_n$ and compute matrix elements of $\widetilde{K}$ and $\widetilde{T}$. Both tasks can be performed simultaneously using the following recursion:

$$\xi_{i+1} = \beta_{i+1}^{-1}(T\eta_i - \alpha_i\xi_i - \beta_i\xi_{i-1}) \tag{8a}$$

$$\eta_{i+1} = \delta_{i+1}^{-1}(K\xi_i - \gamma_i\eta_i - \delta_i\eta_{i-1}). \tag{8b}$$

The four coefficients α_i, β_i, γ_i, and δ_i are to be chosen at each step i such as to make ξ_{i+1} orthogonal to η_i and η_{i-1}, and η_{i+1} – orthogonal to ξ_i and ξ_{i-1}. This appears to be enough to ensure global biorthogonality $(\xi_i\eta_j) = \delta_{ij}$.

Indeed, assume biorthogonality to hold up to step i. Multiplying (8a) by η_j, $j < i-1$, we have $(\eta_j\xi_{i+1}) \propto (\eta_j T\eta_i) = (\eta_i T\eta_j) = 0$ due to Hermiticity of T and the fact that $T\eta_j$ is a linear combination of all ξ_k with $k \leq j+1 < i$. Thus, the biorthogonality also holds for the step $i+1$.

Multiplying (8a) by η_{i-1}, η_i, and η_{i+1} and using biorthogonality, we get $(\xi_i\eta_i) = 1$, $\widetilde{K}_{ii} = \alpha_i$, and $\widetilde{K}_{i,i-1} = \widetilde{K}_{i-1,i} = \beta_i$. Similarly, $\widetilde{T}_{ii} = \gamma_i$ and $\widetilde{T}_{i,i-1} = \widetilde{T}_{i-1,i} = \delta_i$. All other matrix elements of $\widetilde{K}$ and $\widetilde{T}$ vanish.

The recursion (8) is a straightforward generalization of the Hermitian Lanczos recursion [2, 4]

$$\psi_{i+1} = \beta_{i+1}^{-1}(H\psi_i - \alpha_i\psi_i - \beta_i\psi_{i-1}) \tag{9}$$

applicable to any Hermitian matrix H. When $K = T$ and $\xi_1 = \eta_1$ both eq.(8) coincide with each other and with equation (9), up to the notation.

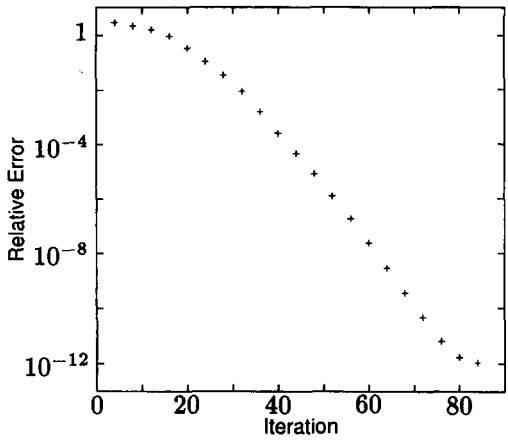
As in the case of the Hermitian Lanczos algorithm, several lowest frequencies can be found one by projecting the ξ- and η-components of converged eigenvectors out of $\mathcal{V}_n$ and $\mathcal{U}_n$ subspaces respectively.

The method was tested on a set of large sparse random matrices of the form (3). Symmetric matrices T and K were generated to have an average of 40 randomly distributed and randomly positioned matrix elements in each row. Both K and T were shifted by an appropriate constant to ensure positive definiteness. Figure demonstrates the convergence results for a matrix of the size $2N = 200000$.

For smaller matrices up to $2N = 2000$, where it was possible to obtain all eigenvalues with regular methods, the present method has converged to the true lowest frequency in all instances.

In conclusion, the method is proposed that generalizes Rayleigh-Ritz variational procedure and Lanczos recursion to the case of non-Hermitian matrices of the form (3), that determine normal modes and frequencies of small-amplitude oscillations of Hamiltonian systems.

Eq.(2) have numerous applications beyond purely mechanical problems. Schroedinger equation in non-orthogonal basis represents a generalized symmetric eigenvalue problem similar to (1). RPA and other time-dependent techniques in nuclear physics and quantum chemistry lead to the equations similar to (2) [3, 5]. At last, eigenvectors of so-called



Convergence of the generalized Lanczos algorithm for a random matrix of the form (3) and size $2N = 200000$

Hamiltonian matrices, to which (3) is a special case, solve the nonlinear algebraic Riccati equation which appears in the theory of stability and optimal control [6].

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