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Error Bounds for Eigenvalues of Unconstrained Structures

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Introduction

THE methods of Krylov-Bogoliubov and Kato-Temple (to be referred to as the Krylov and Kato methods, respectively) for determination of the bounds on natural frequencies are generalized in this Note to the case of an unconstrained mechanical system. The eigenfrequencies ω and eigenvectors x of free vibrations of a discretized elastic system are defined as the solution of the equation

$$Kx = \omega^2 Mx \tag{1}$$

where the stiffness matrix K and the mass matrix M are symmetric and positive definite or semidefinite. Given a certain approximation x_0 of an eigenvector x, the Krylov[1] method supplies the following estimate of the eigenvalue:

$$\frac{1}{\rho+\sqrt{\sigma^2-\rho^2}} \le \omega^2 \le \frac{1}{\rho-\sqrt{\sigma^2-\rho^2}} \tag{2}$$

where

$$\rho = x_0^T M x_0 / x_0^T K x_0 \tag{3}$$

$$\sigma^2 = x_0^T M K^{-1} M x_0 / x_0^T K x_0 \tag{4}$$

Assume that the eigenvalues are numbered in ascending order, as

$$\omega_1^2 \le \omega_2^2 \le \ldots \le \omega_n^2$$

and values μ and ν are known such that $1/\mu$ is an upper bound to ω_{k-1}^2 and $1/\nu$ is a lower bound to ω_{k+1}^2

$$1/\omega_{k+1}^2 \le \nu < \rho < \mu \le 1/\omega_{k-1}^2 \tag{5}$$

Then, the Kato[2] formula can be applied for determination of bounds on eigenvalue ω_k^2 as

$$\frac{1}{\rho+(\sigma^2-\rho^2)/(\rho-\nu)} \le \omega_k^2 \le \frac{1}{\rho+(\sigma^2-\rho^2)/(\rho-\mu)} \tag{6}$$

The Krylov method is usually applied for computation of values μ and ν, which are then used in the Kato formulas, often supplying more restrictive bounds than those of the Krylov method alone. For example, these methods were applied in Refs. 3 and 4 to error estimates of the eigenvalue approximations obtained through the elimination of variables. They may serve as well as reliable termination criteria in iteration methods determining eigenvalues (especially the subspace iteration method).[5]

Since Eq. (4) contains the inverse of the stiffness matrix K, the above formulas can be used only for constrained systems for which K is nonsingular. When a structure and/or its part can undergo displacements as a rigid body (without storing potential deformation energy), its stiffness matrix is singular. In the case of such an unconstrained structure, there are two possibilities of determining error bounds for eigenfrequencies.

The first one can be applied only if the mass matrix M is nonsingular. As the eigenproblem,

$$Mx = (1/\omega^2)Kx \tag{7}$$

is equivalent to Eq. (1) for $\omega \neq 0$, each nonzero eigenfrequency can be estimated by the use of the Krylov and Kato formulas, in which ω is replaced by $1/\omega$ and the roles of K and M are interchanged.

The second method of removing the singularity of K consists in eigenvalue shifting, that is, the addition of the vector $\alpha Mx\,(\alpha > 0)$ to both sides of Eq. (1) leads to the eigenproblem

$$(K+\alpha M)x = (\omega^2+\alpha)Mx \tag{8}$$

In order to apply the methods of Krylov and Kato, the nonsingular matrix $K+\alpha M$ must be inverted.

The aim of this Note is to present an alternative method that uses the flexibility matrix of the system under consideration, one in which the statically determinable constraints (removing all the rigid-body modes) are imposed.

Eigenproblem Formulation for Unconstrained Structure

Suppose that the system has n degrees of freedom, including r rigid-body degrees. Then there exists a matrix R of rigid-body modes, containing r linearly independent columns and satisfying the equation

$$KR = 0 \tag{9}$$

It is easy to notice that the rigid-body modes are the solutions of the eigenproblem represented by Eq. (1) for $\omega = 0$. Besides, there exist $m = n - r$ linearly independent eigenvectors $x_1, x_2, \ldots, x_m$ associated with the nonzero eigenfrequencies and called deformation modes

$$Kx_i = \omega_i^2 Mx_i \quad (i = 1,2,\ldots,m) \tag{10}$$

They are known to have the orthogonality properties, which can be written after suitable normalization as

$$x_i^T K x_j = \delta_{ij} \text{ and } x_i^T M x_j = \lambda_i \delta_{ij} \quad (i,j = 1,\ldots,m) \tag{11}$$

where δ_{ij} is the Kronecker's delta and

$$\lambda_i = 1/\omega_i^2 \quad (\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_m) \tag{12}$$

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Furthermore, the deformation modes are M orthogonal to rigid-body modes

$$R^T M x_i = 0 \quad (i = 1,2,\dots,m) \tag{13}$$

This fundamental fact becomes apparent after multiplication of both sides of Eq. (10) by R^T and taking into account Eq. (9) as well as the fact that $\omega_i \neq 0$.

Denoting with P the projection operator in the direction of the rigid-body modes onto the M orthogonal subspace leads to

$$P = I - R\hat{M}^{-1} R^T M \tag{14}$$

where

$$\hat{M} = R^T M R \tag{15}$$

The following relations result from Eqs. (13–15) and (9):

$$PR = 0 \qquad Px_i = x_i \tag{16}$$

$$P^T M = MP \qquad KP = P^T K = K \tag{17}$$

It has been proved[6–7] that each deformation mode satisfies the equation

$$\lambda_i x_i = PCMx_i \quad (i = 1,2,\dots,m) \tag{18}$$

where λ_i is related to ω_i by Eq. (12) and C is the flexibility matrix of the system on which a set of r statically determinable constraints has been imposed.

Bounds on Eigenvalues

Suppose a vector x_a is an approximation of a certain deformation mode. It can be expanded in terms of all eigenvectors, including the rigid-body modes, as

$$x_a = \sum_{i=1}^{m} \gamma_i x_i + Rz \tag{19}$$

where z is a vector of dimension r. Vector x_0 defined as the projection of x_a in the direction of rigid body nodes onto the M orthogonal subspace,

$$x_0 = Px_a \tag{20}$$

has the following form implied by Eq. (16)

$$x_0 = \sum_{i=1}^{m} \gamma_i x_i \tag{21}$$

Vector x_0 is a better approximation of the eigenvector than x_a because it has no rigid-body components. Being M orthogonal to the rigid-body modes, x_0 satisfies the identity

$$x_0 = Px_0 \tag{22}$$

Using Eqs. (21) and (18), vector w

$$w = PCMx_0 \tag{23}$$

can be put into the form

$$w = \sum_{i=1}^{m} \gamma_i PCMx_i = \sum_{i=1}^{m} \gamma_i \lambda_i x_i \tag{24}$$

Assuming a certain approximation ρ to the eigenvalue, vector v can be defined as

$$v = w - \rho x_0 \tag{25}$$

which, by virtue of Eqs. (24) and (21), can be expressed as

$$v = \sum_{i=1}^{m} (\lambda_i - \rho)\gamma_i x_i \tag{26}$$

Let ϵ^2 be the following scalar quantity:

$$\epsilon^2 = v^T K v / x_0^T K x_0 \tag{27}$$

Assuming that λ_k is an eigenvalue such that

$$|\lambda_k - \rho| = \min_i |\lambda_i - \rho| \tag{28}$$

and taking Eqs. (26), (21), and (11) into consideration results in

$$\epsilon^2 = \sum_{i=1}^{m} \gamma_i^2 (\lambda_i - \rho)^2 \Big/ \sum_{i=1}^{m} \gamma_i^2$$

$$\geq (\lambda_k - \rho)^2 \sum_{i=1}^{m} \gamma_i^2 \Big/ \sum_{i=1}^{m} \gamma_i^2 = (\lambda_k - \rho)^2 \tag{29}$$

Therefore,

$$|1/\omega_k^2 - \rho| \leq \epsilon \tag{30}$$

which is equivalent to the following bounds on an eigenvalue

$$\frac{1}{\rho + \epsilon} \leq \omega_k^2 \leq \frac{1}{\rho - \epsilon} \tag{31}$$

The optimum value of ρ and convenient formula for calculating ϵ can now be derived. Using Eq. (25), the definition of ϵ^2 in Eq. (27) can be put into the form

$$\epsilon^2 = \frac{1}{x_0^T K x_0} \,(w^T K w - 2\rho w^T K x_0 + \rho^2 x_0^T K x_0) \tag{32}$$

According to Eqs. (24), (10), and (21), the product Kw is equal to

$$Kw = \sum_{i=1}^{m} \gamma_i \lambda_i K x_i = \sum_{i=1}^{m} \gamma_i M x_i = Mx_0 \tag{33}$$

Thus,

$$\epsilon^2 = \frac{1}{x_0^T K x_0} \,(x_0^T M w - 2\rho x_0^T M x_0 + \rho^2 x_0^T \mathrm{K} \mathrm{x}_0) \tag{34}$$

It is easy to see that the smallest value of ϵ^2 is attained for the value of ρ defined by Eq. (3) and that

$$\epsilon^2 = \sigma^2 - \rho^2 \tag{35}$$

where

$$\sigma^2 = x_0^T M w / x_0^T K x_0 \tag{36}$$

Equations (23), (17), and (22) imply that

$$\sigma^2 = \frac{x_0^T MPCMx_0}{x_0^T K x_0} = \frac{x_0^T P^T MCMx_0}{x_0^T K x_0} = \frac{x_0^T MCMx_0}{x_0^T K x_0} \tag{37}$$

Using Eqs. (20) and (17), the formulas for ρ and σ can be represented in terms of x_a as

$$\rho = \frac{x_a^T P^T M P x_a}{x_a^T K x_a} \tag{38}$$

$$\sigma^2 = \frac{x_a^T P^T MCMP x_a}{x_a^T P^T K P x_a} = \frac{x_a^T M P^T C P M x_a}{x_a^T K x_a} \tag{39}$$

We have obtained ultimately Eqs. (38) and (39) or Eqs. (3) and (37) for σ and ρ, which—after substituting into Eqs. (28) and (35)—produce bounds on an eigenvalue of the unconstrained system. Equations (28) and (35) are equivalent to the inequality equation (2) of Krylov, while Eqs. (37-39) extend Eqs. (3) and (4) for ρ and σ.

The next step is to generalize the Kato theorem. With this aim, the following vectors are created:

$$v_1 = w - \alpha x_0 \qquad v_2 = w - \beta x_0 \tag{40}$$

where α and β are such numbers that no eigenvalue λ_i lies between them. Equations (21) and (24) imply that

$$v_1 = \sum_{i=1}^{m} (\lambda_i - \alpha)\gamma_i x_i \qquad v_2 = \sum_{i=1}^{m} (\lambda_i - \beta)\gamma_i x_i \tag{41}$$

which, through Eq. (11), yields

$$v_1^T K v_2 / x_0^T K x_0 = \sum_{i=1}^{m} \gamma_i^2 (\lambda_i - \alpha)(\lambda_i - \beta) \Big/ \sum_{i=1}^{m} \gamma_i^2 \geq 0 \tag{42}$$

This inequality can be rearranged by using Eqs. (3), (33), (36), and (40)

$$\frac{1}{x_0^T K x_0}(w^T K w - \alpha x_0^T K w - \beta w^T K x_0 + \alpha\beta x_0^T K x_0)$$

$$= \sigma^2 - \alpha\rho - \beta\rho + \alpha\beta \geq 0 \tag{43}$$

Numbers μ and ν satisfy Eq. (5), i.e.,

$$\lambda_{k+1} \leq \nu < \rho < \mu \leq \lambda_{k-1} \tag{44}$$

which means that no eigenvalue λ_i lies between ν and λ_k, so $\alpha = \nu$ and $\beta = \lambda_k$ can be substituted into Eq. (43), obtaining

$$\lambda_k \leq \frac{\sigma^2 - \nu\rho}{\rho - \nu} = \rho + \frac{\sigma^2 - \rho^2}{\rho - \nu} \tag{45}$$

Analogously assuming $\alpha = \mu$ and $\beta = \lambda_k$ results in

$$\lambda_k \geq \rho + \frac{\sigma^2 - \rho^2}{\rho - \mu} \tag{46}$$

Combining Eqs. (45), (46), and (12) leads to the inequality equation (6) of Kato with generalized formulas for ρ and σ.

Conclusions

It has been proved in this Note that Eqs. (2-4) and (6) of Krylov and Kato are valid for an unconstrained structure, provided that the eigenvector approximation x_0 satisfies Eq. (22) and the matrix K^{-1} is replaced—as in Eq. (37)—by the flexibility matrix C of the system subjected to a minimum number of constraints that remove the rigid-body motion. If an eigenvector approximation x_a is not M orthogonal to the rigid-body modes and therefore does not satisfy Eq. (22), it should be replaced by the vector x_0 according to Eq. (20) or else Eqs. (38) and (39) for ρ and σ should be used instead of Eqs. (3) and (37).

Although matrix C appears in Eqs. (37) and (39), the value of σ is independent of the choice of the constraints used for determining matrix C. This results from Eqs. (36) and (24), which show that σ can be expressed as a function of the values γ_i, which are unique coefficients of expansion of the vector x_a in terms of the eigenvectors. The fact that in Eq. (39) the value of σ is constant for different C can be explained by the constancy of matrix $P^T C P$, while the invariability of σ in Eq. (37) is a consequence of Eq. (22) being imposed on x_0.

It should be stressed that C and P, which are full matrices of dimension n, need not be given explicitly, because only a multiplication of a vector by these matrices need be computed in order to determine ρ and σ. Multiplication of a vector by the matrix C can be performed by using the lower triangular matrix L (usually band) obtained from the Cholesky decomposition of the stiffness matrix of the system with constraints. Matrix L is also useful for computation of the matrix R. Calculation of Px_a can be founded on Eq. (16) by

$$P x_a = x_a - R\hat{M}^{-1}(MR)^T x_a \tag{47}$$

(matrix MR of dimension $n \times r$ was formed during the determination of $\hat{M}$).

The method presented here is an extension of the theorems of Krylov and Kato, but it is not just a trick for avoiding the singularity of the stiffness matrix—as in the case of the alternative methods based on Eqs. (7) and (8). Its advantage occurs when the matrices P and C (or rather R and L) are known—for example, are computed during determination of the eigenvector approximations. It has been successfully applied for estimating the error of eigenvalue approximations obtained as a result of elimination of variables of an unconstrained structure.[8] It can also be used easily for determination of eigenvalue error at each step of the subspace iteration method based on Eq. (18).

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