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On the shift-invert Lanczos method for the buckling eigenvalue problem

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Abstract

We consider the problem of extracting a few desired eigenpairs of the buckling eigenvalue problem $Kx = \lambda K_G x$, where K is symmetric positive semi-definite, K_G is symmetric indefinite, and the pencil $K - \lambda K_G$ is singular, namely, K and K_G share a nontrivial common nullspace. Moreover, in practical buckling analysis of structures, bases for the nullspace of K and the common nullspace of K and K_G are available. There are two open issues for developing an industrial strength shift-invert Lanczos method: (1) the shift-invert operator $(K - \sigma K_G)^{-1}$ does not exist or is extremely ill-conditioned, and (2) the use of the semi-inner product induced by K drives the Lanczos vectors rapidly toward the nullspace of K, which leads to a rapid growth of the Lanczos vectors in norms and causes permanent loss of information and the failure of the method. In this paper, we address these two issues by proposing a generalized buckling spectral transformation of the singular pencil $K - \lambda K_G$ and a regularization of the inner product via a low-rank updating of the semi-positive definiteness of K. The efficacy of our approach is demonstrated by numerical examples, including one from industrial buckling analysis.

KEYWORDS

buckling analysis, eigenvalue problem, Lanczos method, shift-invert, singular pencil

1 | INTRODUCTION

We consider the buckling eigenvalue problem

$$Kx = \lambda K_G x, \tag{1}$$

where K and K_G are $n \times n$ sparse symmetric matrices, and K is positive semi-definite and K_G is indefinite. Furthermore, the pencil $K - \lambda K_G$ is singular, that is, the matrices K and K_G share a nontrivial common nullspace $\mathcal{Z}_c$. We are interested in (i) extracting a few nonzero finite eigenvalues around a prescribed shift $\sigma \neq 0$ and the associated eigenvectors x perpendicular to the common nullspace $\mathcal{Z}_c$, and (ii) counting the number of eigenvalues of $K - \lambda K_G$ in a given interval (α, β). As in practical buckling analysis of structures, we assume that a basis $Z \equiv [Z_N\ Z_C]$ of the nullspace of K and a basis Z_C of the common nullspace $\mathcal{Z}_c$ of K and K_G are available, and the pencil $K - \lambda K_G$ is simultaneously diagonalizable.

The buckling eigenvalue problem (1) arises from the buckling analysis in structural engineering, where K is referred to as the stiffness matrix and K_G is referred to as the geometric stiffness matrix. The eigenvalue λ is used to determine the critical load at which a structure may become unstable (Reference 1, p. 433), and the eigenvector x is the associated buckling shape. The bases for the nullspace of K and the common nullspace $\mathcal{Z}_c$ of K and K_G can be extracted from the algebraic or geometric structure of the problem.[1-3]

The buckling eigenvalue problem (1) remains an outstanding computational challenge in numerical linear algebra[4,5] and in industrial applications.[6] When the pencil $K - \lambda K_G$ is regular and K is positive definite, a common practice for computing eigenpairs around a given shift σ is to convert (1) into the following ordinary eigenproblem via a so-called buckling spectral transformation

$$(K - \sigma K_G)^{-1} K x = \frac{\lambda}{\lambda - \sigma} x, \tag{2}$$

see References [7-10]. Since $(K - \sigma K_G)^{-1} K$ is symmetric with respect to K, the Lanczos method with K-inner product can be immediately used to solve the eigenproblem (2). This approach is referred to as the shift-invert Lanczos method and has been widely used, including in a number of industrial strength eigensolvers, such as LS-DYNA.[6]

However, when K is positive semi-definite and $K - \lambda K_G$ is singular, we have the following two issues:

1. Since the pencil $K - \lambda K_G$ is singular or near singular, that is, the matrices K and K_G share a nontrivial common nullspace $\mathcal{Z}_c$, the shift-invert matrix $(K - \sigma K_G)^{-1}$ does not exist or is extremely ill-conditioned.
2. Since the matrix K is positive semi-definite, the inner product induced by K causes the Lanczos vectors driven rapidly toward the nullspace of K.[4,5,8,11] It results in the large norms of the Lanczos vectors, which introduces large rounding errors. The accuracy of the computed solutions degrades and the procedure can even fail.

These issues have been studied since the early development of the shift-invert Lanczos method in the 1980s. Nour-Omid et al.[8] proposed a modified formulation of the Ritz vectors to refine the computed solutions. Meerbergen[4] proposed to control the norms of the Lanczos vectors by applying implicit restart.[12] More recently, Stewart[5] gave a detailed analysis to show that the loss of information caused by the growth of the Lanczos vectors is permanent.

One way to address the issues is to consider constraints on the degrees of freedom (Reference 1, p. 272). By removing the redundant degrees of freedom, the buckling eigenvalue problem (1) can be transformed into an equivalent symmetric definite generalized eigenvalue problem. This approach, however, could significantly increase the number of nonzero entries in the shifted matrix, leading to huge amount of memory for the factorization. The constraints can also be imposed by augmenting (1) using the Lagrange formulation.[6] But both the augmented matrices become indefinite and the shift-invert Lanczos method is not applicable. Alternative way is to enforce the Lanczos vectors in the desired subspace by deflation.[8] Still, the stability could be a concern.

In this paper, we address the two issues by first proposing a generalized buckling spectral transformation of the singular pencil $K - \lambda K_G$, and a regularization of the inner product via a low-rank updating of the positive semi-definite matrix K. Then a shift-invert Lanczos method for the buckling eigenvalue problem (1) is developed. We will discuss implementation of the matrix-vector product for the computational kernel of the shift-invert Lanczos method, and propose way to count the number of eigenvalues in a given interval (α, β) for validation.

The rest of the paper is organized as follows. In Section 2, we first present a canonical form of the pencil $K - \lambda K_G$, and propose a generalized buckling spectral transformation, and a regularization of the inner product. In Section 3, we discuss the implementation of the shift-invert Lanczos method with the generalized buckling spectral transformation and the regularized inner product. In Section 4, we discuss way to count the number of eigenvalues in an interval. Efficacy of the proposed approach is demonstrated in Section 5. Concluding remarks are given in Section 6.

Following the convention of matrix computations, we use the upper case letters for matrices and lower case letters for vectors. In particular, we use I_n for the identity matrix of dimension n with e_j being the jth column. If not specified, the dimensions of matrices and vectors conform to the dimensions used in the context. $\cdot^T$ is for transpose, $\cdot^\dagger$ for pseudo-inverse, $\|\cdot\|_1$ for 1-norm, and $\|\cdot\|_2$ and $\|\cdot\|_F$ for 2-norm and Frobenius norm, respectively. Also, $\kappa_2(\cdot)$ is for the 2-norm condition number. We use A^{-T} for the inverse of the matrix A^T. The range and the nullspace of a matrix A are denoted by $\mathcal{R}(A)$ and $\mathcal{N}(A)$, respectively. The direct sum of two subspaces $\mathcal{S}_1$ and $\mathcal{S}_2$ is denoted by $\mathcal{S}_1 \oplus \mathcal{S}_2$. The orthogonal complement to a subspace $\mathcal{S}$ is denoted by $\mathcal{S}^\perp$ and the orthogonal projection onto a subspace $\mathcal{S}$ is denoted by $\mathcal{P}_\mathcal{S}$. $\nu_+(S)$, $\nu_-(S)$ and $\nu_0(S)$ denote the numbers of positive, negative and zero eigenvalues of a symmetric matrix S, respectively. Other notations will be explained as used.

2 | THEORY

2.1 | Canonical form

We start with a canonical form of the pencil $K - \lambda K_G$. For the compactness of presentation, we interchange the roles of K and K_G in (1) and consider the reversal of the pencil $K - \lambda K_G$, that is, $K_G - \lambda^\# K$.

Theorem 1. *For the pencil $K_G - \lambda^\# K$, there exists a nonsingular matrix $W \in \mathbb{R}^{n\times n}$ such that*

$$W^T K_G W = \begin{array}{c c} & \begin{array}{ccc} n_1 & n_2 & n_3 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \\ n_3 \end{array} & \begin{bmatrix} \Lambda_1^\# & & \\ & \Lambda_2^\# & \\ & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad W^T K W = \begin{array}{c c} & \begin{array}{ccc} n_1 & n_2 & n_3 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \\ n_3 \end{array} & \begin{bmatrix} I_{n_1} & & \\ & 0 & \\ & & 0 \end{bmatrix} \end{array}, \tag{3}$$

where $\Lambda_1^\#$ and $\Lambda_2^\#$ are diagonal matrices with real diagonal entries, and $\Lambda_2^\#$ is nonsingular. Furthermore, by conformally partitioning $W = [W_1, W_2, W_3]$, we have

$$W_3^T W_1 = 0 \quad \text{and} \quad W_3^T W_2 = 0, \tag{4}$$

Proof. see Appendix A. ∎

Remark 1. By the canonical form (3), we immediately know that (i) the columns of W_3 span the common nullspace $\mathcal{Z}_c$ of K and K_G, and the columns of $[W_1\ W_2]$ span the orthogonal complement to $\mathcal{Z}_c$, that is, $\mathcal{Z}_c^\perp$; (ii) the columns of W_1 are eigenvectors associated with real finite eigenvalues $(\Lambda_1^\#, I_{n_1})$ of the pencil $K_G - \lambda^\# K$ and are perpendicular to $\mathcal{Z}_c$; (iii) The columns of W_2 are eigenvectors associated with an infinite eigenvalue $(\Lambda_2^\#, 0)$ of the pencil $K_G - \lambda^\# K$ and are perpendicular to $\mathcal{Z}_c$; (iv) For $x \in \mathcal{Z}_c$, $(\lambda^\#, x)$ is an eigenpair of the pencil $K_G - \lambda^\# K$ for any $\lambda^\# \in \mathbb{C}$.

2.2 | Generalized buckling spectral transformation

Mathematically, a generalized buckling spectral transformation of the singular pencil $K - \lambda K_G$ is to replace the inverse in (2) by the pseudo-inverse and leads to the ordinary eigenvalue problem

$$Cx = \mu x \quad \text{with} \quad C = (K - \sigma K_G)^\dagger K, \tag{5}$$

where $(K - \sigma K_G)^\dagger$ is the pseudo-inverse of the singular matrix $K - \sigma K_G$ (Reference 13, p. 290). Note that the nonzero real shift σ cannot be an eigenvalue of the pencil $K - \lambda K_G$.

We now present the relationship of nontrivial eigenpairs between the original buckling eigenvalue problem (1) and the ordinary eigenvalue problem (5). We first use the canonical form (3) to derive an eigenvalue decomposition of C and provide the eigenvalue and eigenvector relations between C and $K_G - \lambda^\# K$.

Lemma 1. *With the canonical form (3) in Theorem 1, an eigenvalue decomposition of the matrix C defined in (5) is given by*

$$CW = W \begin{bmatrix} (I_{n_1} - \sigma\Lambda_1^\#)^{-1} & & \\ & 0 & \\ & & 0 \end{bmatrix}. \tag{6}$$

Proof. Recall that, since the matrix $K - \sigma K_G$ is symmetric,

$$\mathcal{R}(K - \sigma K_G) = \mathcal{N}(K - \sigma K_G)^\perp = \mathcal{Z}_c^\perp. \tag{7}$$

In addition, by the condition (4) in the canonical form (3), we have

$$\mathcal{R}(W_1) \oplus \mathcal{R}(W_2) = \mathcal{R}(W_3)^{\perp} = \mathcal{Z}_c^{\perp}. \tag{8}$$

Therefore, from (7) and (8),

$$\mathcal{R}(K - \sigma K_G) = \mathcal{R}(W_1) \oplus \mathcal{R}(W_2) = \mathcal{R}(W_3)^{\perp} = \mathcal{Z}_c^{\perp}. \tag{9}$$

Now note that, from the canonical form (3),

$$W^T K W = \begin{bmatrix} I_{n_1} & & \\ & 0 & \\ & & 0 \end{bmatrix} \quad \text{and} \quad W^T (K - \sigma K_G) W = \begin{bmatrix} I_{n_1} - \sigma \Lambda_1^{\#} & & \\ & -\sigma \Lambda_2^{\#} & \\ & & 0 \end{bmatrix}. \tag{10}$$

Therefore, we have

$$W^T K W = \begin{bmatrix} I_{n_1} & & \\ & 0 & \\ & & 0 \end{bmatrix} = W^T (K - \sigma K_G) W \begin{bmatrix} (I_{n_1} - \sigma \Lambda_1^{\#})^{-1} & & \\ & 0 & \\ & & 0 \end{bmatrix}. \tag{11}$$

Left multiplying (11) by $(K - \sigma K_G)^{\dagger} W^{-T}$,

$$(K - \sigma K_G)^{\dagger} K W = (K - \sigma K_G)^{\dagger} (K - \sigma K_G) W \begin{bmatrix} (I_{n_1} - \sigma \Lambda_1^{\#})^{-1} & & \\ & 0 & \\ & & 0 \end{bmatrix}. \tag{12}$$

The pseudo-inverse $(K - \sigma K_G)^{\dagger}$ satisfies the Moore–Penrose conditions (Reference 13, p. 290), which give

$$(K - \sigma K_G)^{\dagger} (K - \sigma K_G) = \mathcal{P}_{\mathcal{R}((K-\sigma K_G)^T)} = \mathcal{P}_{\mathcal{R}(K-\sigma K_G)}, \tag{13}$$

namely $(K - \sigma K_G)^{\dagger}(K - \sigma K_G)$ is an orthogonal projection onto $\mathcal{R}((K - \sigma K_G)^T) = \mathcal{R}(K - \sigma K_G)$. Therefore, from (9) and (13),

$$(K - \sigma K_G)^{\dagger} (K - \sigma K_G) W = W \begin{bmatrix} I_{n_1} & & \\ & I_{n_2} & \\ & & 0 \end{bmatrix}. \tag{14}$$

From Equations (12) and (14), we have the eigenvalue decomposition (6) of C. ∎

Lemma 2. *The matrix C defined in (5) has the following properties:*

(i) $(\lambda^{\#}, x)$ is an eigenpair of $K_G - \lambda^{\#} K$ with nonzero finite $\lambda^{\#}$ and $x \in \mathcal{Z}_c^{\perp}$ if and only if (μ, x) is an eigenpair of C with $\mu \neq 0$ and $\mu \neq 1$ and $x \in \mathcal{Z}_c^{\perp}$, where $\mu = \frac{1}{1-\sigma\lambda^{\#}}$.
(ii) $(\lambda^{\#}, x)$ is an eigenpair of $K_G - \lambda^{\#} K$ with $\lambda^{\#} = 0$ and $x \in \mathcal{Z}_c^{\perp}$ if and only if (μ, x) is an eigenpair of C with $\mu = 1$ and $x \in \mathcal{Z}_c^{\perp}$.
(iii) $(\lambda^{\#}, x)$ is an eigenpair of $K_G - \lambda^{\#} K$ with $|\lambda^{\#}| = \infty$ and $x \in \mathcal{Z}_c^{\perp}$ if and only if (μ, x) is an eigenpair of C with $\mu = 0$ and $x \in \mathcal{Z}_c^{\perp}$.
(iv) If $x \in \mathcal{Z}_c$, $Cx = 0$.

Proof. The lemma can be proved by comparing the eigenvalue decomposition (6) of C with the canonical form (3) of $K_G - \lambda^{\#} K$. Specifically, for (i) and (ii), recall that each column of W_1 is an eigenvector associated with a real, finite eigenvalue $\lambda^{\#}$ of the pencil $K_G - \lambda^{\#} K$ and the eigenvector is perpendicular to the common nullspace $\mathcal{Z}_c$. From (6), each column of W_1 is now an eigenvector associated with a non-zero, finite eigenvalue $\mu = (1 - \sigma\lambda^{\#})^{-1}$ of the eigenproblem (5).

To show (iii), recall that each column of W_2 is an eigenvector associated with an infinite eigenvalue of the pencil $K_G - \lambda^\# K$ and the eigenvector is perpendicular to the common nullspace $\mathcal{Z}_c$. From (6), each column of W_2 is now an eigenvector associated with zero eigenvalue of the eigenproblem (5).

Finally, for (iv), the common nullspace $\mathcal{Z}_c$ is spanned by the columns of W_3 and, from (6), we know that $Cx = 0$ if $x \in \mathcal{Z}_c$. ■

The following theorem provides the relationship of nontrivial eigenpairs between the original buckling eigenvalue problem (1) and the ordinary eigenvalue problem (5).

Theorem 2. *(λ, x) is an eigenpair of the pencil $K - \lambda K_G$ with nonzero finite eigenvalue λ and $x \in \mathcal{Z}_c^\perp$ if and only if (μ, x) is an eigenpair of the matrix C in (5) with $\mu \neq 0$ and $\mu \neq 1$ and $x \in \mathcal{Z}_c^\perp$, where $\mu = \frac{\lambda}{\lambda - \sigma}$ and $\sigma \neq 0$.*

Proof. Note that (λ, x) is an eigenpair of $K - \lambda K_G$ with nonzero finite eigenvalue λ and $x \in \mathcal{Z}_c^\perp$ if and only if $(\lambda^\#, x)$ is an eigenpair of $K_G - \lambda^\# K$ with non-zero finite eigenvalue $\lambda^\# = \lambda^{-1}$ and $x \in \mathcal{Z}_c^\perp$. Also, from Lemma 2 (i), we know that $(\lambda^\#, x)$ is an eigenpair of $K_G - \lambda^\# K$ with nonzero finite eigenvalue $\lambda^\#$ and $x \in \mathcal{Z}_c^\perp$ if and only if (μ, x) is an eigenpair of the eigenvalue problem $Cx = \mu x$ with $\mu = \frac{1}{1 - \sigma\lambda^\#}$, $\mu \neq 0$ and $\mu \neq 1$, and $x \in \mathcal{Z}_c^\perp$. Therefore, (λ, x) is an eigenpair of the pencil $K - \lambda K_G$ with nonzero finite eigenvalue λ and $x \in \mathcal{Z}_c^\perp$ if and only if (μ, x) is an eigenpair of the eigenvalue problem $Cx = \mu x$ with $\mu = \frac{\lambda}{\lambda - \sigma}$, $\mu \neq 0$ and $\mu \neq 1$, and $x \in \mathcal{Z}_c^\perp$. □

By Theorem 2, near the shift σ, the eigenpairs (λ, x) of $K - \lambda K_G$ with non-zero finite eigenvalues λ and $x \in \mathcal{Z}_c^\perp$ are transformed into eigenpairs (μ, x) of C with nonzero eigenvalues μ, which typically are well-separated, and those away from the shift σ are transformed into clustered eigenpairs (μ, x) of C near unity as shown in Figure 1. We note that the eigenpairs (μ, x) with $\mu = 0$ or $\mu = 1$ are not the ones of interest. The eigenpairs $(1, x)$ correspond to eigenpairs of $K - \lambda K_G$ with infinite eigenvalues and the eigenpairs $(0, x)$ correspond to eigenpairs of $K - \lambda K_G$ with $x \in \mathcal{N}(K)$. ■

2.3 | Regularization of the inner product

In this subsection we introduce a positive definite matrix M from a low-rank updating of K, and then show that the matrix C in the generalized buckling spectral transformation (5) is symmetric with respect to the inner product induced by M.

Theorem 3. *Let C be defined in (5). Let $Z = [Z_N\ Z_C]$ span the nullspace $\mathcal{N}(K)$ and Z_C span the common nullspace $\mathcal{Z}_c$ of K and K_G. Define*

$$M = K + (K_G Z_N) H_N (K_G Z_N)^T + Z_C H_C Z_C^T, \tag{15}$$

where H_N and H_C are arbitrary positive definite matrices. Then

(i) *the matrix M is positive definite,*
(ii) *the matrix C is symmetric with respect to the inner product induced by M.*

Proof. By the canonical form (3), we have

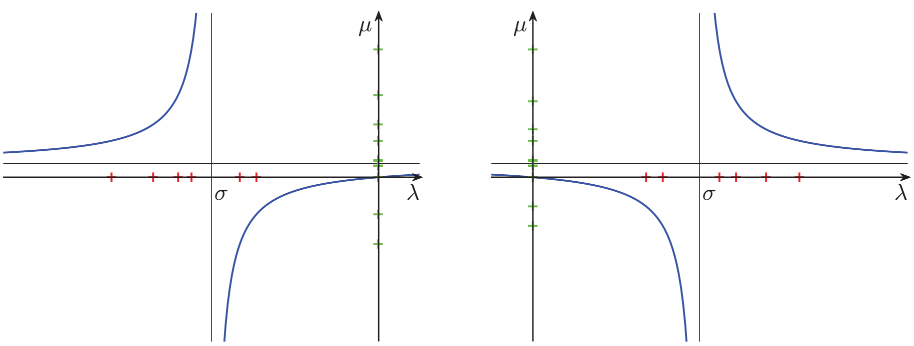


FIGURE 1 Buckling spectral transformation with $\sigma < 0$ (left) and $\sigma > 0$ (right)

$$\mathcal{N}(K) = \mathcal{R}(W_2) \oplus \mathcal{R}(W_3) = \mathcal{R}(Z_N) \oplus \mathcal{R}(Z_C) \quad \text{and} \quad \mathcal{Z}_c = \mathcal{R}(W_3) = \mathcal{R}(Z_C),$$

and

$$\begin{bmatrix} Z_N & Z_C \end{bmatrix} = \begin{bmatrix} W_2 & W_3 \end{bmatrix} \begin{bmatrix} R_{22} & O \\ R_{32} & R_{33} \end{bmatrix},$$

for some matrices $R_{22} \in \mathbb{R}^{n_2 \times n_2}$, $R_{32} \in \mathbb{R}^{n_3 \times n_2}$, $R_{33} \in \mathbb{R}^{n_3 \times n_3}$, and R_{22} and R_{33} are nonsingular. Therefore,

$$W^T K_G Z_N = W^T K_G (W_2 R_{22} + W_3 R_{32}) = W^T K_G W_2 R_{22} = \begin{bmatrix} 0 \\ \Lambda_2^{\#} R_{22} \\ 0 \end{bmatrix}.$$

Since the basis W satisfies the condition (4),

$$W^T Z_C = W^T W_3 R_{33} = \begin{bmatrix} 0 \\ 0 \\ (W_3^T W_3) R_{33} \end{bmatrix}.$$

Therefore,

$$W^T M W = W^T \left(K + (K_G Z_N) H_N (K_G Z_N)^T + Z_C H_C Z_C^T \right) W = \begin{bmatrix} I_{n_1} & & \\ & \hat{H}_N & \\ & & \hat{H}_C \end{bmatrix}, \tag{16}$$

where

$$\hat{H}_N = \Lambda_2^{\#} R_{22} H_N R_{22}^T \Lambda_2^{\#} \quad \text{and} \quad \hat{H}_C = (W_3^T W_3) R_{33} H_C R_{33}^T (W_3^T W_3).$$

To prove that M is positive definite, we show that both $\hat{H}_N$ and $\hat{H}_C$ are positive definite. For the matrix $\hat{H}_N$, we note that the matrix H_N is positive definite and the matrix R_{22} is nonsingular. Also, from Theorem 1, the diagonal matrix $\Lambda_2^{\#}$ is nonsingular. Therefore, the matrix $\hat{H}_N$ is positive definite. For the matrix $\hat{H}_C$, we note that the matrix H_C is positive definite and the matrix R_{33} is nonsingular. Also, since the matrix W_3 is of full rank, the symmetric matrix $W_3^T W_3$ is nonsingular. Therefore, the matrix $\hat{H}_C$ is also positive definite. This proves (i).

To prove (ii), by the eigenvalue decomposition (6) of C and (16), we have

$$W^T M C W = W^T M W W^{-1} C W = \begin{bmatrix} (I_{n_1} - \sigma \Lambda_1^{\#})^{-1} & & \\ & 0 & \\ & & 0 \end{bmatrix}.$$

Therefore, the matrix MC is symmetric, which means that the matrix C is symmetric with respect to the inner product induced by M. ■

Remark 2. We note that if the pencil $K - \lambda K_G$ is regular, Theorem 3 is still applicable. In this case, the matrix C in (2) is symmetric with respect to the inner product induced by $M = K + (K_G Z_N) H_N (K_G Z_N)^T$.

3 | SHIFT-INVERT LANCZOS METHOD

3.1 | Shift-invert Lanczos method

Using Theorem 2, we have generalized the buckling spectral transformation to the singular pencil $K - \lambda K_G$ and converted the buckling eigenproblem (1) into an equivalent ordinary eigenvalue problem (5). From Theorem 3, we know that the matrix C in (5) is symmetric with respect to the inner product induced by the positive definite matrix M in (15). It naturally leads that to solve the buckling eigenvalue problem (1), we can use the Lanczos method on the matrix C with the inner product induced by M. This new strategy is also referred to as the shift-invert Lanczos method and outlined in Algorithm 1.

The shift-invert Lanczos method, after j steps, computes a sequence of Lanczos vectors $\{v_1 \ \dots \ v_{j+1}\}$ and a symmetric tridiagonal matrix $T_j = \text{tridiag}(\beta_{i-1}, \alpha_i, \beta_i)$ satisfying the governing equations

$$CV_j = V_j T_j + \beta_j v_{j+1} e_j^T \quad \text{and} \quad V_{j+1}^T M V_{j+1} = I_{j+1}, \tag{17}$$

where $V_{j+1} \equiv [v_1 \ \dots \ v_{j+1}]$. Care must be taken to ensure that the equations in (17) are satisfied[7-9,14,15] in the presence of finite-precision arithmetic. In particular, at step 11 of Algorithm 1, we perform full re-orthogonalization at each iteration using the classical Gram–Schmidt process (Reference 16, p. 120), that is,

$$r = r - V_j(V_j^T(Mr)).$$

Efficient practical techniques such as partial and selective re-orthogonalization have been developed and well-implemented.[9,14,15] In next subsection, we will focus on the implementation of the matrix-vector product $u = Cv$ at step 6.

Algorithm 1. Shift-invert Lanczos method for the buckling eigenvalue problem (1)

This algorithm takes as input the starting vector v, the matrix-vector product $u = Cv$, the matrix M with the positive definite matrices H_N and H_C, and the tolerance value *tol* for the relative residual norm. It returns the converged eigenpairs $(\hat{\mu}_i, \hat{x}_i)$ of C.

1: $r = v$
2: $p = Mr$
3: $\beta_0 = (p^T r)^{1/2}$
4: **for** $j = 1, 2, \dots$ **do**
5: $\quad v_j = r/\beta_{j-1}$
6: $\quad r = Cv_j$ (see Section 3.2)
7: $\quad r = r - \beta_{j-1} v_{j-1}$
8: $\quad p = Mr$
9: $\quad \alpha_j = v_j^T p$
10: $\quad r = r - \alpha_j v_j$
11: $\quad$ perform re-orthogonalization if necessary
12: $\quad p = Mr$
13: $\quad \beta_j = (p^T r)^{1/2}$
14: $\quad$ compute the eigenpairs $(\hat{\mu}_i, \hat{s}_i)$ of $T_j = \text{tridiag}(\beta_{i-1}, \alpha_i, \beta_i)$
15: $\quad$ use *tol* to check the relative residual norm (33) for convergence
16: **end for**
17: return the converged eigenpairs $(\mu_i, \hat{x}_i = V_j \hat{s}_i)$

3.2 | The matrix-vector product

We first show that the matrix-vector product $u = Cv = (K - \sigma K_G)^{\dagger} K v$ is connected with the solution of a consistent singular linear system with constraint.

Theorem 4. *Given $v \in \mathbb{R}^n$, the vector*

$$u = (K - \sigma K_G)^{\dagger} K v, \tag{18}$$

is the unique solution of the consistent singular linear system

$$(K - \sigma K_G)u = Kv, \tag{19}$$

with the constraint

$$Z_C^T u = 0, \tag{20}$$

where Z_C is a basis of the common nullspace of K and K_G.

Proof. First note that since both K and $K - \sigma K_G$ are symmetric, we have

$$\mathcal{R}(K) = \mathcal{N}(K)^{\perp} \quad \text{and} \quad \mathcal{R}(K - \sigma K_G) = \mathcal{N}(K - \sigma K_G)^{\perp} = \mathcal{Z}_c^{\perp}, \tag{21}$$

and

$$\mathcal{Z}_c = \mathcal{N}(K - \sigma K_G) \subset \mathcal{N}(K). \tag{22}$$

Therefore from (21) and (22),

$$Kv \in \mathcal{R}(K) \subset \mathcal{R}(K - \sigma K_G),$$

which implies that the linear system (19) is consistent. From (18),

$$(K - \sigma K_G)u = (K - \sigma K_G)(K - \sigma K_G)^{\dagger} Kv = \mathcal{P}_{\mathcal{R}(K-\sigma K_G)} Kv = Kv, \tag{23}$$

where $\mathcal{P}_{\mathcal{R}(K-\sigma K_G)}$ is an orthogonal projection onto $\mathcal{R}(K - \sigma K_G)$ (by the Moore–Penrose conditions Reference 13, p. 290). This means that u is a solution of the consistent singular linear system (19).

On the other hand, from (18) and (23),

$$u = (K - \sigma K_G)^{\dagger} Kv = (K - \sigma K_G)^{\dagger}(K - \sigma K_G)u = \mathcal{P}_{\mathcal{R}((K-\sigma K_G)^T)} u = \mathcal{P}_{\mathcal{R}(K-\sigma K_G)} u. \tag{24}$$

Since $\mathcal{R}(K - \sigma K_G) = \mathcal{Z}_c^{\perp}$, it implies that u is perpendicular to the common nullspace $\mathcal{Z}_c$, which is also the nullspace $\mathcal{N}(K - \sigma K_G)$.

The uniqueness can be shown as follows. Given two solutions u_1 and u_2 to (19), the difference $u_1 - u_2$ would satisfy $(K - \sigma K_G)(u_1 - u_2) = 0$, which implies $u_1 - u_2 \in \mathcal{Z}_c$. However, since both solutions satisfy the constraint (20), $Z_C^T(u_1 - u_2) = 0$. Therefore, $u_1 - u_2 = 0$. ■

We now present method to compute the matrix-vector product $u = Cv$. First, we have the following theorem to extract a non-singular submatrix of $K - \sigma K_G$ by exploiting the basis Z_C.

Theorem 5. *Let $Z_C \in \mathbb{R}^{n \times n_3}$ be a basis of $\mathcal{N}(K - \sigma K_G)$ and $P \in \mathbb{R}^{n \times n}$ be a permutation matrix such that $P^T Z_C \equiv \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix}$, and $Y_2 \in \mathbb{R}^{n_3 \times n_3}$ is nonsingular. Define*

$$S = P^T(K - \sigma K_G)P \quad \text{and} \quad S = \begin{array}{c c} & \begin{array}{cc} n-n_3 & n_3 \end{array} \\ \begin{array}{c} n-n_3 \\ n_3 \end{array} & \begin{bmatrix} S_{11}^{\sigma} & S_{12} \\ S_{12}^T & S_{22} \end{bmatrix} \end{array}. \tag{25}$$

Then

(1) the submatrix $S_{11}^{\sigma} \in \mathbb{R}^{(n-n_3)\times(n-n_3)}$ is nonsingular,

(2) $\nu_+(S_{11}^\sigma) = \nu_+(K - \sigma K_G)$ *and* $\nu_-(S_{11}^\sigma) = \nu_-(K - \sigma K_G)$*, where* $\nu_+(X)$ *and* $\nu_-(X)$ *denote the numbers of positive and negative eigenvalues of the symmetric matrix* X*, respectively.*

Proof. Let

$$E = \begin{array}{cc} & \begin{array}{cc} n-n_3 & n_3 \end{array} \\ \begin{array}{c} n-n_3 \\ n_3 \end{array} & \begin{bmatrix} I_{n-n_3} & Y_1 \\ 0 & Y_2 \end{bmatrix} \end{array} \in \mathbb{R}^{n\times n}.$$

The matrix E is non-singular since Y_2 is nonsingular. By the congruence transformation, we have

$$E^T S E = E^T P^T (K - \sigma K_G) P E = E^T \begin{bmatrix} S_{11}^\sigma & S_{12} \\ S_{12}^T & S_{22} \end{bmatrix} E = \begin{array}{cc} & \begin{array}{cc} n-n_3 & n_3 \end{array} \\ \begin{array}{c} n-n_3 \\ n_3 \end{array} & \begin{bmatrix} S_{11}^\sigma & 0 \\ 0 & 0 \end{bmatrix} \end{array}. \tag{26}$$

Sylvester's law (Reference 13, p. 448) tells that the matrices $K - \sigma K_G$ and $E^T S E$ have the same inertias. In particular, from (26), we know that

$$\nu_+(K - \sigma K_G) = \nu_+(S_{11}^\sigma), \quad \nu_-(K - \sigma K_G) = \nu_-(S_{11}^\sigma),$$

and

$$\nu_0(K - \sigma K_G) = \nu_0(S_{11}^\sigma) + n_3 \tag{27}$$

But $\nu_0(K - \sigma K_G) = \dim(\mathcal{N}(K - \sigma K_G)) = n_3$. Therefore, from (27), $\nu_0(S_{11}^\sigma) = 0$ and S_{11}^σ is nonsingular. ■

Theorem 5 was inspired by Reference 17, theorem 2.2, where the authors consider solving a consistent semi-definite linear systems $Ax = b$ from the electromagnetic applications.[18] The matrix A, generated from the finite element modeling, is positive semi-definite and an explicit basis of the nullspace of A is available. This explicit basis of the nullspace is then used to identify a nonsingular part of A and a solution of the linear system can be computed from it. Although in the buckling eigenvalue probem (1), the matrix $K - \sigma K_G$ is indefinite, we found that the strategy developed in Reference 17 can be generalized to the system (19) and (20).

By Theorem 5, the method to solve (19), that is, compute the matrix-vector product $u = Cv = (K - \sigma K_G)^\dagger K v$, can be described in two steps:

1. Find a solution u_p of the consistent singular linear system (19).
2. Compute $u = \mathcal{P}_{\mathcal{R}(K-\sigma K_G)} u_p$ to satisfy the constraint (20), where $\mathcal{P}_{\mathcal{R}(K-\sigma K_G)}$ is an orthogonal projection onto $\mathcal{R}(K - \sigma K_G)$.

Specifically, in Step 1, find the permutation matrix P as described in Theorem 5, and rewrite (19) in the partitioned form (25):

$$\begin{bmatrix} S_{11}^\sigma & S_{12} \\ S_{12}^T & S_{22} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \in \mathcal{R}(S), \tag{28}$$

where

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \equiv P^T u \quad \text{and} \quad \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \equiv P^T K v.$$

Since S_{11}^σ is nonsingular, S_{11}^σ is of full rank and the leading $n - n_3$ columns of S are linearly independent. On the other hand, we know that $\operatorname{rank}(S) = \operatorname{rank}(K - \sigma K_G) = n - n_3$. Therefore, the leading $n - n_3$ columns of S is a basis of $\mathcal{R}(S)$, and there is a solution w_p of (28) with $w_2 = 0$. Direct substitution gives

$$w_p = \begin{bmatrix} (S_{11}^{\sigma})^{-1} c_1 \\ 0 \end{bmatrix},$$

where the inverse $(S_{11}^{\sigma})^{-1}$ can be computed using the sparse LDL^T factorization of S_{11}^{σ}.[19,20] A solution u_p of (19) is then given by

$$u_p = P \begin{bmatrix} (S_{11}^{\sigma})^{-1} c_1 \\ 0 \end{bmatrix}.$$

In Step 2, since Z_C is a basis of $\mathcal{N}(K - \sigma K_G)$, which is the orthogonal complement to $\mathcal{R}(K - \sigma K_G)$, the vector u can be computed by the projection

$$u = \mathcal{P}_{\mathcal{R}(K-\sigma K_G)} u_p = (I - Z_C (Z_C^T Z_C)^{-1} Z_C^T) u_p.$$

If Z_C is an orthonormal basis, then

$$u = \mathcal{P}_{\mathcal{R}(K-\sigma K_G)} u_p = (I - Z_C Z_C^T) u_p.$$

4 | COUNTING EIGENVALUES

In this section, as a validation scheme, we discuss a way to count the number of eigenvalues in a given interval. In the following, $\nu_+(A)$ and $\nu_-(A)$ denote the number of positive and negative eigenvalues of a symmetric matrix A, respectively. $n(\alpha, \beta)$ and $n^\#(\alpha, \beta)$ denote the numbers of eigenvalues of the pencil $K - \lambda K_G$ and the reversed pencil $K_G - \lambda^\# K$ in an interval (α, β), respectively.

First, we consider the following lemma.

Lemma 3. *Let $Z = [Z_N\ Z_C]$ span the nullspace $\mathcal{N}(K)$ and Z_C span the common nullspace $\mathcal{Z}_c$ of K and K_G, then*

(*i*) *for $\alpha < 0$, $n(\alpha, 0) = \nu_-(K - \alpha K_G) - \nu_-(Z_N^T K_G Z_N)$,*
(*ii*) *for $\alpha > 0$, $n(0, \alpha) = \nu_-(K - \alpha K_G) - \nu_+(Z_N^T K_G Z_N)$.*

In addition, the matrix $Z_N^T K_G Z_N$ is nonsingular.

Proof. The proof is based on the following two facts: (1) (λ, x) is an eigenpair of the pencil $K - \lambda K_G$ with nonzero finite eigenvalue λ and $x \in \mathcal{Z}_c^\perp$ if and only if $(\lambda^\#, x)$ is an eigenpair of the pencil $K_G - \lambda^\# K$ with nonzero finite eigenvalue $\lambda^\# = \lambda^{-1}$ and $x \in \mathcal{Z}_c^\perp$. (2) By the canonical form (3), we have

$$W^T \left(K_G - \frac{1}{\alpha} K \right) W = \begin{bmatrix} \Lambda_1^\# - \frac{1}{\alpha} I_{n_1} & & \\ & \Lambda_2^\# & \\ & & 0 \end{bmatrix}.$$

Consequently, by Sylvester's law, we have

$$\nu_-\left(K_G - \frac{1}{\alpha} K \right) = \nu_-\left(\Lambda_1^\# - \frac{1}{\alpha} I_{n_1} \right) + \nu_-(\Lambda_2^\#),$$
$$\nu_+\left(K_G - \frac{1}{\alpha} K \right) = \nu_+\left(\Lambda_1^\# - \frac{1}{\alpha} I_{n_1} \right) + \nu_+(\Lambda_2^\#).$$

Now, for (i), since $\alpha < 0$,

$$n(\alpha, 0) = n^\#\left(-\infty, \frac{1}{\alpha} \right) = \nu_-\left(\Lambda_1^\# - \frac{1}{\alpha} I_{n_1} \right) = \nu_-\left(K_G - \frac{1}{\alpha} K \right) - \nu_-(\Lambda_2^\#) = \nu_-(K - \alpha K_G) - \nu_-(\Lambda_2^\#), \tag{29}$$

where for the second equality, see Remark 1. For (ii), since $\alpha > 0$,

$$n(0,\alpha) = n^{\#}\left(\frac{1}{\alpha}, +\infty\right) = \nu_+\left(\Lambda_1^{\#} - \frac{1}{\alpha} I_{n_1}\right) = \nu_+\left(K_G - \frac{1}{\alpha}K\right) - \nu_+(\Lambda_2^{\#}) = \nu_-(K - \alpha K_G) - \nu_+(\Lambda_2^{\#}). \tag{30}$$

On the other hand, by the canonical form (3), we have

$$\mathcal{N}(K) = \mathcal{R}(Z_N) \oplus \mathcal{R}(Z_C) = \mathcal{R}(W_2) \oplus \mathcal{R}(W_3) \quad \text{and} \quad \mathcal{Z}_c = \mathcal{R}(Z_C) = \mathcal{R}(W_3),$$

and

$$Z_N = W_2 R_{22} + W_3 R_{32},$$

where $R_{22} \in \mathbb{R}^{n_2 \times n_2}$, $R_{32} \in \mathbb{R}^{n_3 \times n_2}$ and R_{22} is nonsingular. Also, we know that $W_2^T K_G W_2 = \Lambda_2^{\#}$. Therefore,

$$Z_N^T K_G Z_N = R_{22}^T (W_2^T K_G W_2) R_{22} = R_{22}^T \Lambda_2^{\#} R_{22}.$$

This implies that the matrix $Z_N^T K_G Z_N$ is nonsingular, and by Sylvester's law, we have

$$\nu_-(\Lambda_2^{\#}) = \nu_-(Z_N^T K_G Z_N) \quad \text{and} \quad \nu_+(\Lambda_2^{\#}) = \nu_+(Z_N^T K_G Z_N). \tag{31}$$

The lemma is an immediate consequence of (29), (30), and (31). ■

Lemma 3 establishes the relation between the number of eigenvalues in the interval $(\alpha, 0)$ or $(0, \alpha)$ and the inertia $\nu_-(K - \alpha K_G)$. Below, we discuss how to express the inertia $\nu_-(K - \alpha K_G)$ in terms of the submatrix S_{11}^{α} in (25).

Lemma 4. *In terms of the submatrix S_{11}^{α} in (25),*

$$\nu_-(K - \alpha K_G) = \nu_-(S_{11}^{\alpha}). \tag{32}$$

Proof. The equality (32) immediately follows from Theorem 5. ■

Combining Lemmas 3 and 4, we have the following theorem which provides a computational approach to count the number of eigenvalues of $K - \lambda K_G$ using the inertias of S_{11}^{α}.

Theorem 6. *In terms of the submatrix S_{11}^{α} in (25), we have*

(*i*) $n(\alpha, 0) = \nu_-(S_{11}^{\alpha}) - \nu_-(Z_N^T K_G Z_N)$, *if* $\alpha < 0$.
(*ii*) $n(0, \alpha) = \nu_-(S_{11}^{\sigma}) - \nu_+(Z_N^T K_G Z_N)$, *if* $\alpha > 0$.

Remark 3. In practice, the inertia $\nu_-(S_{11}^{\alpha})$ is a by-product of the sparse LDL$^{\mathrm{T}}$ factorizations of the submatrix S_{11}^{α} (Reference 21, p. 214). The inertias $\nu_-(Z_N^T K_G Z_N)$ and $\nu_+(Z_N^T K_G Z_N)$ can be easily computed since the size of $Z_N^T K_G Z_N$ is typically small in buckling analysis.

5 | NUMERICAL EXAMPLES

In this section, we begin with a synthetic example to illustrate the issue associated with the growth of the norms of the Lanczos vectors with K-inner product and the consequence of the growth as discussed by Meerbergen[4] and Stewart.[5] Then we demonstrate the efficacy of the proposed shift-invert Lanczos method for an example arising in industrial buckling analysis of structures.

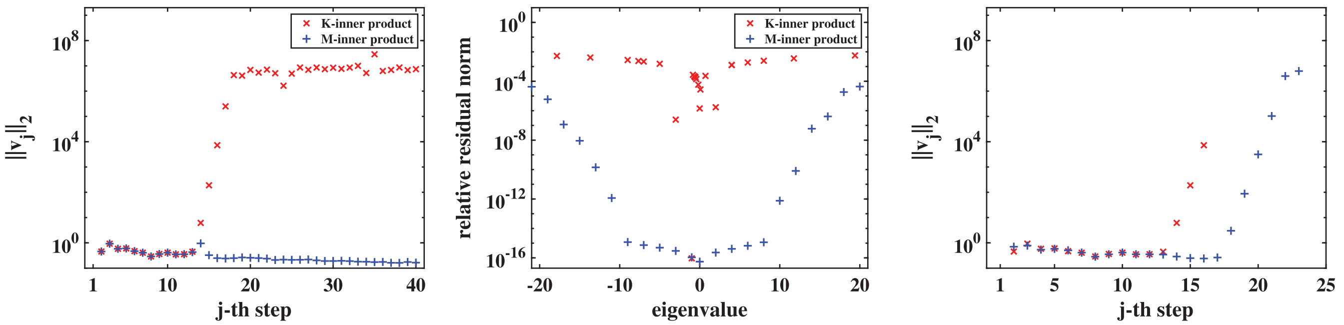


FIGURE 2 Left: the 2-norms of the Lanczos vectors v_j. Middle: the relative residual norms of the approximate eigenpairs $(\hat{\lambda}_i, \hat{x}_i)$. Right: the 2-norms of the Lanczos vectors v_j with (+) and without (x) implicit restart

Algorithm 1 is implemented in MATLAB.[a] The accuracy of a computed eigenpair $(\hat{\lambda}_i, \hat{x}_i)$ of the buckling eigenvalue problem (1) is measured by the relative residual norm

$$\eta(\hat{\lambda}_i, \hat{x}_i) \equiv \frac{\|K\hat{x}_i - \hat{\lambda}_i K_G \hat{x}_i\|_2}{(\|K\|_1 + |\hat{\lambda}_i| \|K_G\|_1)\|\hat{x}_i\|_2}. \tag{33}$$

The Euclidean angle $\theta_i = \angle(\hat{x}_i, \mathcal{Z}_c)$ is computed for checking if $\hat{x}_i$ is perpendicular to the common nullspace $\mathcal{Z}_c$ of K and K_G.[22,23]

Example 1. Let us consider the following matrix pair (K, K_G) similar to the ones constructed by Meerbergen[4] and Stewart:[5]

$$K = Q\Lambda Q^T \in \mathbb{R}^{n\times n} \quad \text{and} \quad K_G = Q\Phi Q^T \in \mathbb{R}^{n\times n},$$

where $Q \in \mathbb{R}^{n\times n}$ is a random orthogonal matrix, $\Lambda \in \mathbb{R}^{n\times n}$ and $\Phi \in \mathbb{R}^{n\times n}$ are diagonal matrices with diagonal elements

$$\Lambda_{kk} = \begin{cases} k, & \text{if} \quad 1 \le k \le n-m \\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad \Phi_{kk} = (-1)^k, \quad 1 \le k \le n.$$

By construction, K is positive semi-definite and K_G is indefinite, and the pencil $K - \lambda K_G$ is regular. The last m columns of Q form a basis of the nullspace $\mathcal{N}(K)$. For $1 \le k \le n-m$, the kth column of Q is an eigenvector and the associated eigenvalue is $\lambda_k = (-1)^k \cdot k$. The zero eigenvalue of $C \equiv (K - \sigma K_G)^{-1}K$ is a well-separated eigenvalue, and the associated eigenspace is also the nullspace of K. We use the MATLAB function `ldl` to compute the LDL$^{\mathrm{T}}$ factorization of the shifted matrix $K - \sigma K_G$.

For numerical experiments, we take $n = 500$ and $m = 1$. We use the buckling spectral transformation (2) with the shift $\sigma = -0.6$. We run the Lanczos method with K-inner product, and the starting vector Cx_0 with $x_0 = [1, \ \dots, \ 1]^T$. The approximate eigenpairs $(\hat{\lambda}_i, \hat{x}_i)$ of (1) are computed by $(\hat{\lambda}_i, \hat{x}_i) = \left(\frac{\sigma\hat{\mu}_i}{\hat{\mu}_i - 1}, \hat{x}_i\right)$.

The left plot of Figure 2 shows the 2-norms of 40 Lanczos vectors v_j. As observed by Meerbergen[4] and Stewart,[5] the 2-norms of Lanczos vectors v_j grow rapidly. Consequently, as shown in the middle plot of Figure 2, the accuracy of approximate eigenpairs $(\hat{\lambda}_i, \hat{x}_i)$ deteriorates. In contrast, when we replace the K-inner product by the positive definite M-inner product with $H_N = I_m$, we observe that the 2-norms of the Lanczos vectors are well bounded. Multiple eigenvalues near the shift σ are computed with the relative residual norms around the machine precision.

We note that in Reference 4, Meerbergen proposed to control the norms of the Lanczos vectors by applying implicit restart. We experimented the schemes with and without the implicit restart The results are shown in the right plot of Figure 2. We can see that the 2-norms of the Lanczos vectors still grow rapidly.

[a]An implementation is available at https://github.com/cplin722/bucklingEigs.

Example 2. This is an example from the buckling analysis of a finite element model of an airplane shown in Figure 3. The size of the pencil $K - \lambda K_G$ is $n = 67,512$. The stiffness matrix K is positive semi-definite and the dimension of the nullspace $\mathcal{N}(K)$ is known to be 6, which corresponds to the six rigid body modes.[2] The geometric stiffness matrix K_G is symmetric but indefinite. The basis Z of $\mathcal{N}(K)$ is computed by $Z = [-(K_{11}^{-1}K_{12})^T \; I_6]^T$,[2] where $[K_{11} \; K_{12}] \in \mathbb{R}^{(n-6)\times n}$ is the leading block rows of K. The dimension of the common nullspace $\mathcal{Z}_c$ of K and K_G is 3, which can be easily computed from the basis Z, see Reference 13, theorem 6.4.1). The accuracy of the bases is shown in the table in Figure 3. We are interested in computing the nonzero eigenvalues of the pencil $K - \lambda K_G$ in an interval around zero and the associated eigenvectors perpendicular to the common nullspace $\mathcal{Z}_c$.

We use the method to compute the matrix-vector product $u = Cv$ described in Section 3.2. We determine the permutation matrix P by maximizing the number of nonzero entries in the last n_3 columns of S in (25). The MATLAB function `ldl`, which uses MA57[24] for real sparse matrices, is used to compute the sparse $\mathrm{LDL^T}$ factorization of the submatrix S_{11}^{σ}. The pivot tolerance $\tau = 0.1$ is used to control the numerical stability of the factorization.[24] In defining the positive definite matrix M, we form the product K_GZ_N and normalize each column of the matrices K_GZ_N and Z_C. The condition number of K_GZ_N after the normalization is $\kappa_2(K_GZ_N) = 1.03$. Then we set the matrices $H_N = \omega I_{n_2}$ and $H_C = \omega I_{n_3}$, $\omega = \|K\|_1$, to balance the matrix M.[25] The starting vector of the Lanczos procedure is $v = Cx_0$ with x_0 being a random vector.[8]

To monitor the progress of the shift-invert Lanczos method, an approximate eigenpair $(\hat{\mu}_i, \hat{x}_i)$ computed from an eigenpair $(\hat{\mu}_i, \hat{s}_i)$ of the reduced matrix T_j is considered to have converged if the following two conditions are satisfied:

$$|\hat{\mu}_i| \geq \text{tol} \quad \text{and} \quad \frac{|\sigma|}{(\hat{\mu}_i - 1)^2}|\beta_j||e_j^T\hat{s}_i| < \text{tol}, \tag{34}$$

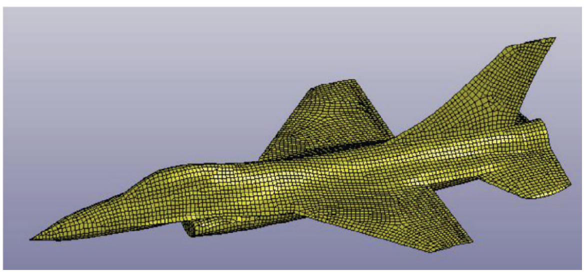
where the first condition excludes the zero eigenvalues and the second condition bounds the error of the computed eigenvalue $\hat{\lambda}_i = \frac{\sigma\hat{\mu}_i}{\hat{\mu}_i - 1}$ with the prescribed tolerance *tol* (see References 7,9, and 26, p. 357). In this numerical example, we experiment with the tolerance $\text{tol} = 10^{-6}$.

We now show the numerical results for computing nonzero eigenvalues of the pencil $K - \lambda K_G$ and corresponding eigenvectors perpendicular to the common nullspace $\mathcal{Z}_c$ in the interval $(-8, 8)$. First, let us consider the left-half interval $(-8, 0)$. With the shift $\sigma = -4.0$, the shift-invert Lanczos method (Algorithm 1) computed 12 eigenvalues to the machine precision in the interval $(-8, 0)$ at 38th iteration. The accuracy of the computed eigenpairs $\left(\hat{\lambda}_i = \frac{\sigma\hat{\mu}_i}{\hat{\mu}_i - 1}, \hat{x}_i\right)$ is shown in Table 1. To validate the number of eigenvalues in the interval $(-8, 0)$, we use the counting scheme described in Section 4. Using the inertias of the submatrix S_{11}^{α} with $\alpha = -8$ and Theorem 5, we have

$$n(-8, 0) = \nu_-(S_{11}^{\alpha}) - \nu_-(Z_N^T K_G Z_N) = 15 - 3 = 12.$$

This matches the number of eigenvalues found in the interval.

Next let us consider the right-half interval $(0, 8)$. In this case, we use the shift $\sigma = 4.0$. By the shift-invert Lanczos method (Algorithm 1), we found 13 eigenvalues to the machine precision in the interval $(0, 8)$ at 44th iteration. The accuracy of the computed eigenpairs $\left(\hat{\lambda}_i = \frac{\sigma\hat{\mu}_i}{\hat{\mu}_i - 1}, \hat{x}_i\right)$ are shown in Table 2. To validate the number of eigenvalues in the interval $(0, 8)$, we again use the counting scheme described in Section 4. Using the inertias of the submatrix S_{11}^{α} with $\alpha = 8$ and Theorem 5, we have



i	$d_i/\|K_G\|_1$	$\frac{\|Kz_i\|_2}{\|K\|_1\|z_i\|_2}$	$\frac{\|K_Gz_i\|_2}{\|K_G\|_1\|z_i\|_2}$
1	$6.90 \cdot 10^{-5}$	$2.74 \cdot 10^{-16}$	$6.78 \cdot 10^{-5}$
2	$3.25 \cdot 10^{-5}$	$4.88 \cdot 10^{-16}$	$9.06 \cdot 10^{-6}$
3	$2.32 \cdot 10^{-5}$	$4.71 \cdot 10^{-16}$	$1.19 \cdot 10^{-5}$
4	$7.32 \cdot 10^{-16}$	$2.68 \cdot 10^{-17}$	$5.01 \cdot 10^{-18}$
5	$1.26 \cdot 10^{-16}$	$1.90 \cdot 10^{-17}$	$4.89 \cdot 10^{-18}$
6	$7.81 \cdot 10^{-18}$	$2.37 \cdot 10^{-17}$	$5.00 \cdot 10^{-18}$

FIGURE 3 Left: Finite element model of an airplane. Right: Accuracy of the bases for the nullspace of K and common nullspace of K and K_G. The second column shows the singular values d_i of K_GY with Y being an orthonormal basis of $\mathcal{N}(K)$. The third and fourth columns show the accuracy of the basis $Z = [Z_N \; Z_C] = [z_1 \; z_2 \; \dots \; z_6]$

i	$\hat{\lambda}_i$	$\eta(\hat{\lambda}_i, \hat{x}_i)$	$\cos\angle(\hat{x}_i, \mathcal{Z}_c)$
1	−2.716598	$1.48 \cdot 10^{-17}$	$8.52 \cdot 10^{-17}$
2	−2.883589	$1.73 \cdot 10^{-17}$	$8.27 \cdot 10^{-17}$
3	−3.292700	$1.37 \cdot 10^{-17}$	$4.84 \cdot 10^{-18}$
4	−3.378406	$1.01 \cdot 10^{-17}$	$2.38 \cdot 10^{-17}$
5	−5.754628	$2.72 \cdot 10^{-17}$	$4.04 \cdot 10^{-17}$
6	−5.854071	$2.92 \cdot 10^{-17}$	$3.47 \cdot 10^{-17}$
7	−6.089281	$3.14 \cdot 10^{-17}$	$2.47 \cdot 10^{-17}$
8	−6.228974	$2.67 \cdot 10^{-17}$	$6.24 \cdot 10^{-17}$
9	−6.784766	$5.33 \cdot 10^{-16}$	$4.93 \cdot 10^{-17}$
10	−6.886759	$2.57 \cdot 10^{-15}$	$7.67 \cdot 10^{-18}$
11	−7.561377	$1.88 \cdot 10^{-12}$	$1.31 \cdot 10^{-16}$
12	−7.745144	$3.83 \cdot 10^{-12}$	$4.87 \cdot 10^{-17}$

TABLE 1 Results of 12 computed eigenvalues in the interval $(-8, 0)$ after 38 steps of the Lanczos method with the shift $\sigma = -4.0$. $\|\hat{X}^T M \hat{X} - I_{12}\|_F = 4.75 \cdot 10^{-12}$ with $\hat{X} \equiv [\hat{x}_1 \ \dots \ \hat{x}_{12}]$

i	$\hat{\lambda}_i$	$\eta(\hat{\lambda}_i, \hat{x}_i)$	$\cos\angle(\hat{x}_i, \mathcal{Z}_c)$
1	2.967043	$3.80 \cdot 10^{-17}$	$1.10 \cdot 10^{-16}$
2	3.025965	$2.96 \cdot 10^{-17}$	$3.39 \cdot 10^{-17}$
3	3.917831	$1.71 \cdot 10^{-17}$	$7.71 \cdot 10^{-17}$
4	4.008941	$1.61 \cdot 10^{-17}$	$7.13 \cdot 10^{-17}$
5	4.591063	$2.43 \cdot 10^{-17}$	$4.29 \cdot 10^{-17}$
6	4.662575	$2.64 \cdot 10^{-17}$	$2.47 \cdot 10^{-17}$
7	5.699271	$5.24 \cdot 10^{-17}$	$7.45 \cdot 10^{-17}$
8	5.725937	$7.44 \cdot 10^{-17}$	$1.38 \cdot 10^{-17}$
9	6.465175	$7.40 \cdot 10^{-16}$	$1.14 \cdot 10^{-16}$
10	6.598173	$7.96 \cdot 10^{-15}$	$2.18 \cdot 10^{-16}$
11	7.285975	$4.45 \cdot 10^{-15}$	$3.32 \cdot 10^{-16}$
12	7.626265	$2.41 \cdot 10^{-14}$	$1.39 \cdot 10^{-15}$
13	7.880296	$1.24 \cdot 10^{-12}$	$3.71 \cdot 10^{-14}$

TABLE 2 Results of 13 computed eigenvalues in the interval $(0, 8)$ after 44 steps of the Lanczos method with the shift $\sigma = 4.0$. $\|\hat{X}^T M \hat{X} - I_{13}\|_F = 1.79 \cdot 10^{-11}$ with $\hat{X} \equiv [\hat{x}_1 \ \dots \ \hat{x}_{13}]$.

$$n(0, 8) = \nu_-(S_{11}^{\alpha}) - \nu_+(Z_N^T K_G Z_N) = 13 - 0 = 13.$$

This also matches the number of computed eigenvalues in the interval.

6 | CONCLUDING REMARK

We studied the buckling eigenvalue problem of singular pencil, and addressed two open issues associated with the shift-invert Lanczos method. We found that the proposed scheme for counting the number of eigenvalues is a reliable tool for validation.

It is still an open problem how to choose the positive definite matrices H_N and H_C for the optimal condition number $\kappa_2(M)$. An analysis following the work in Reference 25 is a direction of future research.

Also note that there are different implementations of the matrix-vector product $u = Cv$. Similar validation schemes can be developed. Performance of different implementations for practical industrial examples is a subject of further study.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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APPENDIX A. CANONICAL FORM OF A SYMMETRIC SEMI-DEFINITE PENCIL $A - \lambda B$

In this section, we give a constructive derivation of a canonical form of a symmetric semi-definite pencil $A - \lambda B$, namely A is symmetric and B is symmetric semi-positive definite.

Theorem 7. *For a symmetric semi-definite pencil $A - \lambda B$, there exists a non-singular matrix $W \in \mathbb{R}^{n\times n}$ such that*

$$W^TAW = \begin{array}{c} \\ 2n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\begin{array}{c} \begin{array}{cccc} 2n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} S & & & \\ & \Lambda_1 & & \\ & & \Lambda_2 & \\ & & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad W^TBW = \begin{array}{c} \\ 2n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\begin{array}{c} \begin{array}{cccc} 2n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} \Omega & & & \\ & I_{n_1} & & \\ & & 0 & \\ & & & 0 \end{bmatrix} \end{array}, \tag{A1}$$

where

$$S \equiv I_{n_0} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \Omega \equiv I_{n_0} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix},$$

Λ_1 and Λ_2 are diagonal matrices with real diagonal entries, and Λ_2 is nonsingular. Moreover, we have

$$\begin{aligned} n_0 &= \dim(\mathcal{N}(B)) - n_2 - n_3, \\ n_1 &= \operatorname{rank}(B) - n_0, \\ n_2 &= \operatorname{rank}(\mathcal{P}_{\mathcal{N}(B)} A \mathcal{P}_{\mathcal{N}(B)}), \\ n_3 &= \dim(\mathcal{N}(A) \cap \mathcal{N}(B)), \end{aligned}$$

where $\mathcal{P}_{\mathcal{N}(B)}$ is the orthogonal projection onto $\mathcal{N}(B)$.

We first introduce the following lemma due to Fix and Heiberger,[27] also see Reference 26, section 15.5.

Lemma 5. *For the symmetric semi-definite pencil $A - \lambda B$, there exists a non-singular matrix $W \in \mathbb{R}^{n\times n}$ such that*

$$W^TAW = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}\begin{array}{c} \begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\ \begin{bmatrix} A_{00} & A_{01} & A_{02} & \Sigma & 0 \\ A_{01}^T & A_{11} & A_{12} & & \\ A_{02}^T & A_{12}^T & \Lambda_2 & & \\ \Sigma & & & 0 & \\ 0 & & & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad W^TBW = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}\begin{array}{c} \begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\ \begin{bmatrix} I_{n_0} & & & & \\ & I_{n_1} & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \end{array},$$

where Λ_2 and Σ are non-singular, diagonal matrices with real diagonal entries.

Proof. Proof of Theorem 7. By Lemma 5, there exists a non-singular matrix $W_0 \in \mathbb{R}^{n\times n}$ such that

$$A^{(1)} \equiv W_0^TAW_0 = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}\begin{array}{c} \begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\ \begin{bmatrix} A_{00} & A_{01} & A_{02} & \Sigma & 0 \\ A_{01}^T & A_{11} & A_{12} & & \\ A_{02}^T & A_{12}^T & \Lambda_2 & & \\ \Sigma & & & 0 & \\ 0 & & & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad B^{(1)} \equiv W_0^TBW_0 = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}\begin{array}{c} \begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\ \begin{bmatrix} I_{n_0} & & & & \\ & I_{n_1} & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \end{array},$$

where Λ_2 and Σ are nonsingular, diagonal matrices with real diagonal entries.

Let

$$
W_1 \equiv \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}
\begin{array}{c}
\begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\
\begin{bmatrix}
I_{n_0} & & & & \\
& I_{n_1} & & & \\
& & I_{n_2} & & \\
-\Sigma^{-1}A_{00}/2 & -\Sigma^{-1}A_{01} & -\Sigma^{-1}A_{02} & I_{n_0} & \\
& & & & I_{n_3}
\end{bmatrix}
\end{array},
$$

then

$$
A^{(2)} \equiv W_1^T A^{(1)} W_1 = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}
\begin{array}{c}
\begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\
\begin{bmatrix}
0 & & & \Sigma & \\
& A_{11} & A_{12} & & \\
& A_{12}^T & \Lambda_2 & & \\
\Sigma & & & 0 & \\
& & & & 0
\end{bmatrix}
\end{array}
\quad \text{and} \quad
B^{(2)} \equiv W_1^T B^{(1)} W_1 = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}
\begin{array}{c}
\begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\
\begin{bmatrix}
I_{n_0} & & & & \\
& I_{n_1} & & & \\
& & 0 & & \\
& & & 0 & \\
& & & & 0
\end{bmatrix}
\end{array}.
$$

Next let

$$
W_2 \equiv \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}
\begin{array}{c}
\begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\
\begin{bmatrix}
I_{n_0} & & & & \\
& I_{n_1} & & & \\
& -\Lambda_2^{-1}A_{12}^T & I_{n_2} & & \\
& & & I_{n_0} & \\
& & & & I_{n_3}
\end{bmatrix}
\end{array},
$$

then

$$
A^{(3)} \equiv W_2^T A^{(2)} W_2 = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}
\begin{array}{c}
\begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\
\begin{bmatrix}
0 & & & \Sigma & \\
& C_{11} & & & \\
& & \Lambda_2 & & \\
\Sigma & & & 0 & \\
& & & & 0
\end{bmatrix}
\end{array}
\quad \text{and} \quad
B^{(3)} \equiv W_2^T B^{(2)} W_2 = \begin{array}{c} \\ n_0 \\ n_1 \\ n_2 \\ n_0 \\ n_3 \end{array}
\begin{array}{c}
\begin{array}{ccccc} n_0 & n_1 & n_2 & n_0 & n_3 \end{array} \\
\begin{bmatrix}
I_{n_0} & & & & \\
& I_{n_1} & & & \\
& & 0 & & \\
& & & 0 & \\
& & & & 0
\end{bmatrix}
\end{array},
$$

where $C_{11} \in \mathbb{R}^{n_1 \times n_1}$ is symmetric and $C_{11} = A_{11} - A_{12}\Lambda_2^{-1}A_{12}^T$.

Define the permutation matrix

$$
P_3 \equiv \begin{bmatrix}
I_{n_0} & 0 & 0 & 0 & 0 \\
0 & 0 & I_{n_1} & 0 & 0 \\
0 & 0 & 0 & I_{n_2} & 0 \\
0 & I_{n_0} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & I_{n_3}
\end{bmatrix},
$$

then

$$A^{(4)} \equiv P_3^T A^{(3)} P_3 = \begin{array}{c} \\ n_0 \\ n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\!\!\begin{array}{c} \begin{array}{ccccc} n_0 & n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} & \Sigma & & & \\ \Sigma & & & & \\ & & C_{11} & & \\ & & & \Lambda_2 & \\ & & & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad B^{(4)} \equiv P_3^T B^{(3)} P_3 = \begin{array}{c} \\ n_0 \\ n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\!\!\begin{array}{c} \begin{array}{ccccc} n_0 & n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} I_{n_0} & & & & \\ & 0 & & & \\ & & I_{n_1} & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \end{array}.$$

Since $C_{11} \in \mathbb{R}^{n_1 \times n_1}$ is symmetric, it admits the eigen-decomposition

$$C_{11} = Q_1 \Lambda_1 Q_1^T,$$

where $Q_1 \in \mathbb{R}^{n_1 \times n_1}$ is an orthogonal matrix and $\Lambda_1 \in \mathbb{R}^{n_1 \times n_1}$ is a diagonal matrix. Applying the congruent transformation associated with $W_4 \equiv \operatorname{diag}(I_{n_0}, \Sigma^{-1}, Q_1, I_{n_2}, I_{n_3})$, we have

$$A^{(5)} \equiv W_4^T A^{(4)} W_4 = \begin{array}{c} \\ n_0 \\ n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\!\!\begin{array}{c} \begin{array}{ccccc} n_0 & n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} & I_{n_0} & & & \\ I_{n_0} & & & & \\ & & \Lambda_1 & & \\ & & & \Lambda_2 & \\ & & & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad B^{(5)} \equiv W_4^T B^{(4)} W_4 = \begin{array}{c} \\ n_0 \\ n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\!\!\begin{array}{c} \begin{array}{ccccc} n_0 & n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} I_{n_0} & & & & \\ & 0 & & & \\ & & I_{n_1} & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \end{array}.$$

Last, define the permutation matrix $P_5 \equiv \operatorname{diag}(E, I_{n_1}, I_{n_2}, I_{n_3})$ with $E \equiv [e_1 \; e_{n_0+1} \; e_2 \; \dots \; e_{2n_0}]$ and we have the canonical form in (A1)

$$A^{(6)} \equiv P_5^T A^{(5)} P_5 = \begin{array}{c} \\ 2n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\!\!\begin{array}{c} \begin{array}{cccc} 2n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} S & & & \\ & \Lambda_1 & & \\ & & \Lambda_2 & \\ & & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad B^{(6)} \equiv P_5^T B^{(5)} P_5 = \begin{array}{c} \\ 2n_0 \\ n_1 \\ n_2 \\ n_3 \end{array}\!\!\begin{array}{c} \begin{array}{cccc} 2n_0 & n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} \Omega & & & \\ & I_{n_1} & & \\ & & 0 & \\ & & & 0 \end{bmatrix} \end{array},$$

where

$$S \equiv I_{n_0} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad \Omega \equiv I_{n_0} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

The canonical form (A1) is obtained with $W \equiv W_0 W_1 W_2 P_3 W_4 P_5$.

Now we interpret the dimension of each block matrix. From the canonical form of B in Equation (A1), we can infer that $n_0 = \dim(\mathcal{N}(B)) - n_2 - n_3$ and $n_1 = \operatorname{rank}(B) - n_0$. Also, $n_3 = \dim(\mathcal{N}(A) \cap \mathcal{N}(B))$. To interpret n_2, let $Z \in \mathbb{R}^{n \times (n_0+n_2+n_3)}$ be the basis of $\mathcal{N}(B)$ consisting of the columns of W and consider the QR decomposition of $Z = QR$. Since Q is an orthonormal basis of $\mathcal{N}(B)$, $\operatorname{rank}(\mathcal{P}_{\mathcal{N}(B)} A \mathcal{P}_{\mathcal{N}(B)}) = \operatorname{rank}(Q^T A Q)$. By the Sylvester's law, $\operatorname{rank}(Q^T A Q) = \operatorname{rank}(Z^T A Z)$. But, from the canonical form (A1), $Z^T A Z = \operatorname{diag}(0_{n_0}, \Lambda_2, 0_{n_3})$ and $\operatorname{rank}(Z^T A Z) = n_2$. Therefore, $n_2 = \operatorname{rank}(\mathcal{P}_{\mathcal{N}(B)} A \mathcal{P}_{\mathcal{N}(B)})$. ■

Corollary 1. *The symmetric semi-definite pencil $A - \lambda B$ is simultaneously diagonalizable if and only if $n_0 = 0$. In this case, we have the canonical form*

$$
W^T A W = \begin{array}{c} \\ n_1 \\ n_2 \\ n_3 \end{array} \begin{array}{c} \begin{array}{ccc} n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} \Lambda_1 & & \\ & \Lambda_2 & \\ & & 0 \end{bmatrix} \end{array} \quad \text{and} \quad W^T B W = \begin{array}{c} \\ n_1 \\ n_2 \\ n_3 \end{array} \begin{array}{c} \begin{array}{ccc} n_1 & n_2 & n_3 \end{array} \\ \begin{bmatrix} I_{n_1} & & \\ & 0 & \\ & & 0 \end{bmatrix} \end{array},
$$

Proof. From the pairs (S, Ω) and $(\Lambda_2, 0)$ in Equation (A1), we note that the algebraic and geometric multiplicity of the infinite eigenvalues are $2n_0 + n_2$ and $n_0 + n_2$, respectively. Therefore, the symmetric semi-definite pencil $A - \lambda B$ is simultaneously diagonalizable if and only if $n_0 = 0$. ■