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A THEORETICAL COMPARISON BETWEEN INNER PRODUCTS IN THE SHIFT-INVERT ARNOLDI METHOD AND THE SPECTRAL TRANSFORMATION LANCZOS METHOD*

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Abstract. The spectral transformation Lanczos method and the shift-invert Arnoldi method are probably the most popular methods for the solution of linear generalized eigenvalue problems originating from engineering applications, including structural and acoustic analyses and fluid dynamics. The orthogonalization of the Krylov vectors requires inner products. Often, one employs the standard inner product, but in many engineering applications one uses the inner product using the mass matrix. In this paper, we make a theoretical comparison between these inner products in the framework of the shift-invert Arnoldi method. The conclusion is that when the square-root of the condition number of the mass matrix is small, the convergence behavior does not strongly depend on the choice of inner product. The theory is illustrated by numerical examples arising from structural and acoustic analyses. The theory is extended to the discretized Navier-Stokes equations.

Key words. Lanczos method, Arnoldi's method, generalized eigenvalue problem, shift-invert.

AMS subject classifications. 65F15.

1. Introduction. This paper is concerned with the solution of generalized eigenvalue problems of the form

$$Ax = \lambda Bx, \qquad A, B \in \boldsymbol{R}^{n\times n}, \qquad x \neq 0\ , \tag{1.1}$$

where A may be symmetric or non-symmetric, and B is symmetric positive (semi) definite, by the spectral transformation Lanczos method [6, 18] and the shift-invert Arnoldi method [17]. Applications include the modal analysis of structures without damping, which leads to

$$Ku = \omega^2 Mu, \tag{1.2}$$

where K and M are symmetric matrices and often positive definite [9]. Typically, the number of wanted eigenmodes for representing the structural properties for low and mid frequencies ranges from a few tens to a few thousands. The modal extraction of acoustic finite element models also leads to a problem of the form (1.2). The required number of eigenmodes is often small, since the modes are usually employed for a low frequency analysis. For the (Navier) Stokes problem, we have

$$\begin{bmatrix} K & C \\ C^T & 0 \end{bmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \lambda \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{pmatrix} u \\ p \end{pmatrix}, \tag{1.3}$$

where M is symmetric positive definite, C is of full rank and K is symmetric (Stokes [14]) or nonsymmetric (Navier-Stokes). This eigenvalue problem arises in the determination of the stability of a steady state solution. Here only the rightmost eigenvalue is wanted [14, 3]. This paper concentrates on the solution of (1.2), but (1.3) will also be touched on. In both applications, M is a discretization of the continuous identity operator, i.e., the continuous inner product $\langle x, y\rangle$ is replaced by the discrete $x^T My$. As a result, the condition number of M is usually small. We study this specific case. The theory is illustrated by numerical examples arising from real applications.

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One approach to the solution of generalized eigenvalue problems is the shift-invert Arnoldi method [17, 20, 15]. Instead of solving (1.1) directly, one solves the shifted and inverted problem

$$(A - \sigma B)^{-1} Bx = \theta x \tag{1.4}$$

by the Arnoldi method. The scalar σ is called the shift, which explains the name 'shift-invert'. If (θ, x) is an eigenpair of $(A - \sigma B)^{-1}B$, then $(\sigma + \theta^{-1}, x)$ is an eigenpair of $Ax = \lambda Bx$. This relation demonstrates that λ's can be computed from θ's. Without loss of generality, we assume a shift $\sigma = 0$ is used. In general, $A^{-1}B$ is a nonsymmetric matrix, even when A and B are symmetric, and this is the reason why the Arnoldi method is used. However, when A is symmetric and B is symmetric positive definite, $A^{-1}B$ is self-adjoint with respect to the B-inner product. This implies that the Lanczos method *can* be used, when the B-inner product $x^T By$ is employed instead of the standard inner product $x^T y$. This idea was proposed by Ericsson [5] and Nour-Omid, Parlett, Ericsson and Jensen [18]. A block version was proposed by Grimes, Lewis and Simon [10]. In the case where B is positive semi-definite, which, e.g. arises in applications of the form (1.3), the B-semi-inner product can be used in the Lanczos method or the Arnoldi method. This is suggested by Ericsson [5], Nour-Omid, Parlett, Ericsson and Jensen [18], and Meerbergen and Spence [16] and applied to linearized and discretized Navier-Stokes equations by Lehoucq and Scott [12].

In this paper, we show by both analysis and numerical examples that if the square root of the condition number of the mass matrix B is small, the choice of inner product does not influence the convergence speed. The choice of inner product should be based on other criteria than rate of convergence. We illustrate this for two classes of applications. When A is symmetric, the use of the B-inner product reduces the Arnoldi method to the Lanczos method. The Lanczos method has two advantages over the Arnoldi method. First, the eigenvalues have quadratic error bounds and their convergence is well understood [19, 20]. Second, the cost per iteration consists of the action of $A^{-1}B$ on a vector and the orthogonalization of the new iteration vector against the previous ones. The cost for the construction of the Krylov basis is smaller than for the Arnoldi method, since only the last two basis vectors are used in the orthogonalization process. The Arnoldi method uses all vectors. The Lanczos method uses the B-inner product which can be quite expensive compared to the standard inner product. The overall orthogonalization cost, however, can be much smaller than for the Arnoldi method with standard inner product, when the number of iteration vectors is large. This is often the case for a structural analysis for low and mid frequencies since a large number of eigenmodes is wanted. The use of the standard inner product instead of the B-inner product may be preferred when A is nonsymmetric and the Arnoldi method needs to be used anyway, so full orthogonalization against all previous basis vectors cannot be avoided. Lehoucq and Scott [12] demonstrate for discretized Navier-Stokes applications that the B-inner product *is* more expensive than the standard inner product, but leads to a more reliable Arnoldi method.

A side effect of the use of B-orthogonalization is that the approximate eigenvectors are B-orthogonal, when A is symmetric. This is very natural since the exact eigenvectors corresponding to different eigenvalues *are* B-orthogonal. In finite element applications, it is assumed that the computed eigenmodes satisfy this property. This is automatically satisfied by the Lanczos method with B-orthogonalization, but not by the Arnoldi method.

The plan of this paper is as follows. In §2, a theoretical comparison between standard and B orthogonalization is established. In §3, we present an easy way of obtaining B-orthogonal eigenvectors from the Arnoldi method when A is symmetric. In §4, we illustrate the theory by numerical examples. Section 5 generalizes the ideas from §2 to the Navier-Stokes problem. Finally, we summarize the main conclusions in §6. We assume computations in exact arithmetic.

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2. A relation between standard and B-orthogonalization. In this section, a theoretical study of the Arnoldi method with standard orthogonalization and B-orthogonalization is established for the eigenvalue problem (1.2). The goal is to relate the residual norms as well as the Hessenberg matrix (which is tridiagonal for the Lanczos method) and the computed eigenvalues for both types of inner product. The analysis assumes exact arithmetic.

First, in §2.1, some preliminaries and notation are presented. Second, §2.2 puts both types of orthogonalization into a single theoretical framework: we present the algorithm and some properties. The relation between standard and B-inner products in the Arnoldi method will be formulated and derived in §2.3.

2.1. Notation and preliminaries. This section is devoted to some notation and matrix properties. In general, we use the Euclidean norm for vectors and matrices, denoted by $\|\cdot\|_2$ or $\|\cdot\|$. The matrix Frobenius norm is denoted by $\|\cdot\|_F$. Let $\kappa(C)$ denote the condition number of the matrix C.

First, since B is a positive definite matrix, there exists $L \in \boldsymbol{R}^{n\times n}$ such that $B = L^T L$.

LEMMA 2.1. *Consider $V, W \in \boldsymbol{R}^{n\times k}$. Let $V^T V = I$, $W^T BW = I$ and let the columns of V span the same space as the columns of W. Then there is an S such that $V = WS$. Moreover, $\kappa(S) = \kappa(W) \leq \sqrt{\kappa(B)}$.*

Proof. It is clear that there is an S such that $V = WS$. Hence $V^T BV = S^T S$ and $W^T W = S^{-T}S^{-1}$. Since $\|V\| = 1$, we have $\|S\|^2 = \|V^T BV\| \leq \|B\|$, and since $W^T BW = (LW)^T(LW) = I$, we have $\|S^{-1}\|^2 = \|W^T W\| = \|(LW)^T B^{-1}(LW)\| \leq \|B^{-1}\|$. This completes the proof. □

We will compare two algorithms that differ primarily in their choice of inner product or norm. We will use the notation $\langle x, y\rangle$ to stand for a generic inner product, such as $x^T y$ or $x^T By$. The notation is also generalized to matrices $V = [v_1, \ldots, v_k]$ and $W = [w_1, \ldots, w_l]$, as follows :

$$\langle V, x\rangle = [\langle v_j, x\rangle]_{j=1}^{k} \in \boldsymbol{R}^k$$
$$\langle W, V\rangle = [\langle w_i, v_j\rangle]_{(i,j)=(1,1)}^{(l,k)} \in \boldsymbol{R}^{l\times k} .$$

Since $\langle\cdot,\cdot\rangle$ is an inner product, it follows that $\langle WS, VZ\rangle = S^T\langle W, V\rangle Z$.

The B norm of a vector x is defined by $\|x\|_B = \sqrt{x^T Bx}$. The B norm of a matrix C is defined by $\|C\|_B = \|LC\|_2$, where $B = L^T L$. Obviously, for two matrices, $V \in \boldsymbol{R}^{n\times k}$ and $W \in \boldsymbol{R}^{n\times l}$, we have $\|V^T BW\| \leq \|V\|_B\|W\|_B$.

For a matrix C, the Krylov space $\mathcal{K}_k(C, v_1)$ of order k with starting vector v_1 is defined by

$$\mathcal{K}_k(C, v_1) = \mathrm{span}\{v_1, Cv_1, C^2 v_1, \ldots, C^{k-1}v_1\} .$$

We assume that all Krylov spaces of order k have dimension k. In practice, a space is represented by a basis. The following lemma gives a relation between two different bases.

LEMMA 2.2. *Let $V_k, W_k \in \boldsymbol{R}^{n\times k}$ be such that the first j columns of V_k and the first j columns of W_k form two bases for $\mathcal{K}_j(C, v_1)$ for $j = 1, .., k$. Then there is a full rank upper triangular matrix $S_k \in \boldsymbol{R}^{k\times k}$ such that $V_k = W_k S_k$.*

The following lemma shows the uniqueness of a normalized Krylov basis.

LEMMA 2.3 (Implicit Q Theorem). *([8, Theorem 7.4.2]) Let the first j columns of V_k and $W_k \in \boldsymbol{R}^{n\times k}$ form two bases for $\mathcal{K}_j(C, v_1)$ for $j = 1, \ldots, k$ and $\langle V_k, V_k\rangle = I = \langle W_k, W_k\rangle$. Then $v_i = w_i\delta_i$ with $\delta_i = \pm 1$ for $i = 1, \ldots, k$.*

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2.2. A general (theoretical) framework for Krylov methods. The Arnoldi and Lanczos methods for the solution of (1.2) are Krylov subspace methods, i.e., the eigenvalues and eigenvectors are computed from the projection of $A^{-1}B$ on a Krylov space. The following algorithm covers both methods. Recall that $\langle x, y\rangle$ denotes the inner product, e.g. the standard inner product $\langle x, y\rangle = x^T y$ or the B-inner product $\langle x, y\rangle = x^T By$.

ALGORITHM 1. *General framework for the Lanczos and Arnoldi methods.*

0. Given v_1 with $\langle v_1, v_1\rangle = 1$.
1. **For** $j = 1$ **to** k **do**
   1.1. Form $p_j = A^{-1}Bv_j$.
   1.2. Compute the Gram Schmidt coefficients $h_{ij} = \langle v_i, p_j\rangle, i = 1, \ldots, j$.
   1.3. Update $q_j = p_j - \sum_{i=1}^{j} v_i h_{ij}$.
   1.4. Compute norm $h_{j+1,j} = \langle q_j, q_j\rangle^{1/2}$.
   1.5. Normalize : $v_{j+1} = q_j / h_{j+1,j}$.
2. Let $\underline{H}_k = [h_{ij}]_{(i,j)=(1,1)}^{(k+1,k)} \in \boldsymbol{R}^{k+1\times k}$ where $h_{ij} = 0$ whenever $i > j + 1$.
   Let H_k be the first k rows of $\underline{H}_k$.
   Let $V_k = [v_1, \ldots, v_k]$.
3. Compute eigenpairs (θ, z) of H_k, with $z \in \boldsymbol{R}^k$, by the QR method.
4. Compute the 'Ritz' vector $x = V_k z \in \boldsymbol{R}^n$.
5. Compute the residual norm $\rho = h_{k+1,k}|e_k^T z|$.

Step 1.1 is performed by a matrix vector multiplication with B and the solution of a linear system with A. The solution of the linear system is usually performed by a direct method, since one can take advantage of the fact that A needs to be factored only once. Moreover, direct methods usually give a solution with a small backward error. This is required for the Arnoldi method to find the eigenpairs of (1.1) [15]. Steps 1.1 to 1.5 compute a basis $V_{k+1} = [v_1, \ldots, v_{k+1}]$ of the Krylov space

$$\mathcal{K}_{k+1}(A^{-1}B, v_1) = \text{span}\{v_1, A^{-1}Bv_1, \ldots, (A^{-1}B)^k v_1\} ,$$

normalized such that $\langle V_{k+1}, V_{k+1}\rangle = I$. The normalization is performed by Gram-Schmidt orthogonalization. For reasons of numerical stability, practical implementations use reorthogonalization [4] in the Arnoldi method and modified Gram-Schmidt with partial reorthogonalization in the Lanczos method [10]. The Gram-Schmidt coefficients are collected in the upper Hessenberg matrix $\underline{H}_k$. Note that $\underline{H}_k$ is a $k + 1$ by k matrix. We denote the $k \times k$ upper submatrix of $\underline{H}_k$ by H_k. By the elimination of p_j and q_j from Steps 1.1 to 1.5, it follows that

$$A^{-1}BV_k = V_{k+1}\underline{H}_k \tag{2.1a}$$
$$= V_k H_k + v_{k+1} h_{k+1,k} e_k^T \ . \tag{2.1b}$$

This is the well known recurrence relation for the Arnoldi and Lanczos methods. Usually, $k \ll n$, so that H_k has much smaller dimensions than A and B. In Steps 3-4, an eigenpair (θ, x) is computed by the Galerkin projection of $A^{-1}B$ on $\mathcal{K}_k$, i.e., $x \in \mathcal{K}_k$ and the residual $r = A^{-1}Bx - \theta x$ is orthogonal to the Krylov space :

$$x = V_k z \quad \text{ with } \quad H_k z = \theta z \ . \tag{2.2}$$

The θ's are the eigenvalues of H_k and are called 'Ritz' values and the x's are the corresponding 'Ritz' vectors. They form an approximate eigenpair of $A^{-1}B$. Recall that H_k is an upper Hessenberg matrix, so the eigenpairs (θ, z) are efficiently computed by the QR method [8, §7.5]. The residual $r = A^{-1}Bx - \theta x$ also follows from (2.1b) :

$$r = A^{-1}Bx - \theta x = v_{k+1} h_{k+1,k} e_k^T z \tag{2.3}$$

and the induced norm is very cheaply computed as

$$\rho = \langle r, r\rangle^{1/2} = h_{k+1,k}|e_k^T z| \ . \tag{2.4}$$

This explains Step 5 in the algorithm. The residual norm is a measure of the accuracy of the eigenvalues. (See eigenvalue perturbation theory, e.g., [20, Ch. III] and [1, Ch. 2].) In the following, we also use a block formulation of the recurrence relation for the 'Ritz' vectors. Let $X_l = [x_1, \ldots, x_l] = V_k Z_l$ and $D_l = \operatorname{diag}(\theta_1, \ldots, \theta_l)$ represent $l \le k$ Ritz pairs and $R_l = [r_1, \ldots, r_l]$ the corresponding residual terms of the form (2.3). Then it follows that

$$A^{-1}BX_l = X_l D_l + R_l , \qquad R_l = h_{k+1,k} v_{k+1} e_k^T Z_l \ . \tag{2.5}$$

In the rest of this paper, we use the following notation to distinguish between the standard and B-orthogonalization. For standard orthogonalization, the Krylov vectors are denoted by V_{k+1} and the Hessenberg matrix is $\underline{H}_k$. They satisfy

$$A^{-1}BV_k = V_{k+1}\underline{H}_k , \qquad \underline{H}_k = V_{k+1}^T A^{-1} B V_k , \qquad V_{k+1}^T V_{k+1} = I \ .$$

For B-orthogonalization, the Krylov vectors are denoted by W_{k+1} and the Hessenberg matrix by $\underline{T}_k$. They satisfy

$$A^{-1}BW_k = W_{k+1}\underline{T}_k , \qquad \underline{T}_k = W_{k+1}^T B A^{-1} B W_k , \qquad W_{k+1}^T B W_{k+1} = I \ .$$

It is clear that if A is symmetric, the Hessenberg matrix $T_k = V_k^T B A^{-1} B V_k$ is symmetric, hence tridiagonal.

2.3. Comparison between both orthogonalization schemes. In this section, a relationship between standard and B-orthogonalization is established. Clearly, the computed Krylov spaces are the same, but the projections differ and this may lead to different eigenvalue approximations. The theoretical result in this section uses Lemma 2.2, which makes the link between two Krylov bases by use of an upper triangular matrix. First, in Theorem 2.4, we relate $h_{k+1,k}$ and $t_{k+1,k}$ and H_k and T_k, and in Theorem 2.5, we relate the eigenvalues of T_k and H_k.

THEOREM 2.4. *Let $v_1 = w_1/\|w_1\|$. Then there is a matrix $S_k \in \boldsymbol{R}^{k\times k}$, such that*

$$\begin{aligned} T_k &= S_k H_k S_k^{-1} + E \\ \|E\|_2 &\le h_{k+1,k}\kappa(W_{k+1}) \end{aligned} \tag{2.6}$$

$$\kappa(W_{k+1})^{-1} \le \frac{t_{k+1,k}}{h_{k+1,k}} \le \kappa(W_{k+1}) \ ,$$

and

$$\kappa(S_k), \kappa(W_{k+1}) \le \sqrt{\kappa(B)} \ .$$

Proof. Recall that V_{k+1} and $\underline{H}_k$ satisfy the Arnoldi recurrence relation (2.1a). Let $S_{k+1} \in \boldsymbol{R}^{k+1\times k+1}$ be the upper triangular Cholesky factor of $V_{k+1}^T B V_{k+1}$, i.e.,

$$V_{k+1}^T B V_{k+1} = S_{k+1}^T S_{k+1} \ .$$

As a consequence, $V_{k+1}S_{k+1}^{-1}$ forms a B-orthogonal Arnoldi basis for the Krylov space. Since Krylov bases are unique (see Lemma 2.3), $W_{k+1} = V_{k+1}S_{k+1}^{-1}$. (Eventually, the columns

S_{k+1} must be multiplied by -1, see δ_i in Lemma 2.3.) The Arnoldi relation (2.1a) can be rewritten as

$$A^{-1}B(V_kS_k^{-1}) = (V_{k+1}S_{k+1}^{-1})(S_{k+1}\underline{H}_kS_k^{-1}),$$

where S_k is the $k \times k$ principle submatrix of S_{k+1}. Consequently, $\underline{T}_k = S_{k+1}\underline{H}_kS_k^{-1}$. Decompose

$$S_{k+1}\underline{H}_kS_k^{-1} = \begin{bmatrix} S_k & s \\ 0 & s_{k+1,k+1} \end{bmatrix} \begin{bmatrix} H_k \\ h_{k+1,k}e_k^T \end{bmatrix} S_k^{-1}$$
$$\underline{T}_k = \begin{bmatrix} T_k \\ t_{k+1,k}e_k^T \end{bmatrix} .$$

Then, we have

$$T_k = S_kH_kS_k^{-1} + E$$

where

(2.7) $$E = h_{k+1,k}s_{k,k}^{-1}se_k^T$$

and

$$t_{k+1,k} = h_{k+1,k}s_{k+1,k+1}s_{k,k}^{-1} .$$

The proof now follows from Lemma 2.1. □

This theorem says that when the square root of the condition number of B is small, the residual terms are of the same order. It also says that T_k is a rank-one update of H_k of the order of $h_{k+1,k}$.

The following theorem establishes a relationship between eigenpairs of T_k and H_k.

THEOREM 2.5. *Let (θ, V_kz) be a 'Ritz' pair of the Arnoldi method and let ρ be the corresponding residual norm. Assume that $v_1 = w_1/\|w_1\|$. Then there exists an eigenvalue η of T_k such that*

$$|\theta - \eta| \leq \kappa(Y_k)\kappa(W_{k+1})\rho ,$$

where Y_k is the matrix whose columns contain the eigenvectors of T_k.

Proof. From (2.6) and the fact that $H_kz = \theta z$, we have

$$S_kH_kz - T_kS_kz = -ES_kz$$
$$T_kS_kz - \theta S_kz = ES_kz .$$

With $y = S_kz/\|S_kz\|$ and $\rho = h_{k+1,k}|e_k^Tz|$, it follows from (2.7) and $e_k^TS_k = s_{k,k}e_k^T$ that

$$\|T_ky - \theta y\| \leq \frac{h_{k+1,k}|s_{k,k}^{-1}|\|s\||e_k^TS_kz|}{\|S_kz\|}$$
$$\leq \frac{h_{k+1,k}\|s\||e_k^Tz|}{\|S_kz\|} = \frac{\|s\|}{\|S_kz\|}h_{k+1,k}|e_k^Tz|$$
(2.8) $$\leq \kappa(S_{k+1})\rho = \kappa(W_{k+1})\rho .$$

Following the Bauer-Fike Theorem [20, Theorem 3.6], it follows that T_k has an eigenvalue η for which

$$|\eta - \theta| \leq \kappa(Y_k)\|T_ky - \theta y\| ,$$

from which the proof follows. □

The eigenvalues of H_k can similarly be related to the eigenvalues of T_k. When A is symmetric, so is T_k. Therefore $\kappa(Y_k) = 1$, and the error bound becomes sharper. The most important conclusion is that the 'Ritz' values with a small residual norm ρ are almost the same for both the standard and the B-inner products.

3. Computation of B-orthogonal eigenvectors in the Arnoldi method. When the B-inner product is used and A and B are symmetric, the tridiagonal matrix T_k is symmetric, so T_k has an orthogonal set of eigenvectors $z_j, j = 1, \ldots, k$. Therefore, the Ritz vectors $W_k z_j$, $j = 1, \ldots, k$ form a B-orthogonal set of k vectors.

When the standard inner product is used, the 'Ritz' vectors are not necessarily B-orthogonal. The following theorem shows the dependence of the B-orthogonality on the separation between the eigenvalues and on the norms of the residuals.

THEOREM 3.1. *Let (θ_j, x_j), $j = 1, \ldots, l < k$ be 'Ritz' pairs and r_j the corresponding residuals computed by the Arnoldi method with the standard inner product. Then, for $1 \leq i, j \leq l$, we have*

$$\frac{|x_i^T B x_j|}{\|x_i\|_B \|x_j\|_B} \leq \frac{\|r_j\|_B / \|x_j\|_B + \|r_i\|_B / \|x_i\|_B}{|\theta_i - \theta_j|} ,$$

provided that $\theta_i \neq \theta_j$.

Proof. Denote by D_l the diagonal matrix containing $\theta_1, \ldots, \theta_l$, and let the columns of X_l be the corresponding Ritz vectors. By multiplying (2.5) on the left by $X_l^T B$, we have

$$X_l^T B A^{-1} B X_l = X_l^T B X_l D_l + X_l^T B R_l \ . \tag{3.1}$$

Since the left-hand side is symmetric,

$$X_l^T B X_l D_l + X_l^T B R_l = D_l X_l^T B X_l + R_l^T B X_l \tag{3.2}$$

and, so

$$X_l^T B X_l D_l - D_l X_l^T B X_l = R_l^T B X_l - X_l^T B R_l \ .$$

The (i, j) element of this matrix leads to the result of the theorem. □

This theorem shows that eigenvectors corresponding to different distinct eigenvalues are almost B-orthogonal, but the eigenvectors corresponding to clustered eigenvalues can lose B-orthogonality. So, an additional B-orthogonalization of the eigenvectors is desirable.

In the following, we use the notations of (2.5), i.e., D_l denotes the diagonal matrix containing $l \leq k$ Ritz values $\theta_1, \ldots, \theta_l$ and the columns of X_l denote the corresponding Ritz vectors. The most robust way to obtain B-orthogonal Ritz vectors, is to compute the B-orthogonal projection of $A^{-1}B$ onto the range of X_l and compute new eigenpairs from this projection. This is established as follows. Let S_l be the upper triangular Cholesky factor of $X_l^T B X_l = S_l^T S_l$. Then, with $Y_l = X_l S_l^{-1}$, we have $Y_l^T B Y_l = I$. A Ritz pair obtained by B-orthogonalization is of the form $(\eta, y = Y_l z)$ with (η, z) satisfying

$$Y_l^T B A^{-1} B Y_l z = \eta z \ . \tag{3.3}$$

This additional projection leads to quadratic error bounds for the eigenvalues. (See e.g. the Kato-Temple theorem [20, Theorem 3.8].) The matrix on the left-hand side of (3.3) can be computed explicitly, but can as well easily be computed without the action of A^{-1} by the use of (3.1) :

$$Y_l^T B A^{-1} B Y_l = S_l D_l S_l^{-1} + Y_l^T B R_l S_l^{-1} \tag{3.4}$$

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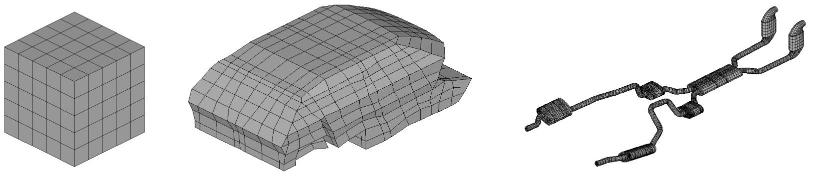

FIG. 4.1. *Meshes for the three eigenvalue problems in §4*

In practice, we could compute (η, z) from

$$(S_l D_l S_l^{-1} + Y_l^T B R_l S_l^{-1}) z = \theta z \tag{3.5}$$

instead of (3.3).

However, there is an alternative to performing an additional projection. The columns of Y_l can be taken as the B-orthogonal 'Ritz' vectors. From the following theorem, it follows that if the residual norms of (θ_j, x_j) for $j = 1, \ldots, l$ are small and $\sqrt{\kappa(B)}$ is small, the residuals for $(\theta_j, Y_l e_j)$ for $j = 1, \ldots, l$ are also small. Of course, the 'Ritz' values do not satisfy a quadratic error bound.

THEOREM 3.2. *Recall the definition of D_l and X_l from Eq. (2.5). Let S_l be the upper triangular Cholesky factor of $X_l^T B X_l$ and let $Y_l = X_l S_l^{-1}$. Then*

$$\|A^{-1} B Y_l - Y_l D_l\|_B \le (\sqrt{l} + 1)\sqrt{\kappa(B)}\|R_l\| \,.$$

Proof. From (3.4), we have

$$Y_l^T B A^{-1} B Y_l = S_l D_l S_l^{-1} + E$$

with $E = Y_l^T B R_l S_l^{-1}$. Since S_l is upper triangular, and D_l diagonal, $S_l D_l S_l^{-1} = D_l + U$ where U is strictly upper triangular. Note that $S_l D_l S_l^{-1} + E$ is symmetric and so is $U + E$: $U + E = U^T + E^T$. This implies

$$\begin{aligned} U - U^T &= E - E^T \\ 2\|U\|_F^2 &\le 2\|E\|_F^2 \end{aligned}$$

and so $\|U\|_2 \le \|E\|_F \le \sqrt{l}\|E\|_2$. From (2.5), we have

$$\begin{aligned} A^{-1} B Y_l - Y_l D_l &= Y_l (S_l D_l S_l^{-1} - D_l) + R_l S_l^{-1} \\ &= Y_l U + R_l S_l^{-1} \\ \|A^{-1} B Y_l - Y_l D_l\|_B &\le \|U\|_2 + \sqrt{\kappa(B)}\|R_l\|_2 \\ &\le (\sqrt{l} + 1)\sqrt{\kappa(B)}\|R_l\|_2 \end{aligned}$$

from which the proof follows. □

4. Numerical examples. All examples have been generated using SYSNOISE, a software tool for vibro-acoustic simulation [22]. The matrices A and B arise from acoustic and structural finite element models and are symmetric. We present results for the following problems.

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PROBLEM 1. The first application concerns the structural modal analysis of a square box with Young modulus $2. \cdot 10^{11}$Pa, Poisson coefficient 0.3 and volume density $7800\,\mathrm{kg/m^3}$. The thickness of the material is 0.01m. One of the six faces of the box is fixed. For the finite element analysis, we used 150 shell elements. This analysis leads to an eigenvalue problem (1.2). For this problem, $A = K$ and $B = M$. The dimension of the problem is $n = 852$ and $\sqrt{\kappa(B)} \approx 1.20 \cdot 10^3$. We used a shift $\sigma = -10$ in the shift-invert transformation of (1.4).

PROBLEM 2. The acoustic modal analysis of a Volvo 480 3D car interior discretized with 744 cubic elements and 68 pentaedral finite elements leads to a problem of the form (1.2) with K positive semi-definite. The fluid has volume density $1.225\,\mathrm{kg/m^3}$ and sound has a speed of 340 m/s (air). For this problem, $A = K$ and $B = M$. The dimension of the problem is $n = 1176$ and $\sqrt{\kappa(B)} \approx 21.2$. We used a shift $\sigma = -10$ in the shift-invert transformation of (1.4).

PROBLEM 3. This concerns the coupling of a structural and an acoustic problem. We consider a square box of 1 m^3 with Young modulus $2. \cdot 10^{11}$Pa, Poisson coefficient 0.3 and volume density $7800\,\mathrm{kg/m^3}$. The thickness of the material is 0.01 m. One of the six faces of the box is fixed. The box is filled with air (speed of sound 340 m/s and volume density $1.29\,\mathrm{kg/m^3}$). The box is discretized by 294 shell elements, which represents the structural model. The acoustic behavior of the fluid is modeled by a boundary element mesh of 294 quadrangular elements. The matrix A is the structural stiffness matrix, while B is the sum of the structural mass matrix and the added mass matrix coming from the acoustic model. The dimension of the problem is $n = 1692$ and $\sqrt{\kappa(B)} \approx 1.2 \cdot 10^3$. A shift $\sigma = 0$ was used.

PROBLEM 4. The acoustic modal analysis of a Jaguar X100MS exhaust pipe discretized with 39254 cubic finite elements leads to a problem of the form (1.2) with K positive semi-definite. The fluid has volume density $1.225\mathrm{kg/m^3}$ and the sound has a speed of 340 m/s (air). The dimension of the problem is $n = 46966$ and $\sqrt{\kappa(B)} \approx 42.8$. For this problem, $A = K$ and $B = M$. The shift σ is chosen such that the 11 dominant eigenvalues of $(A - \sigma B)^{-1}B$ correspond to the eigenfrequencies between 0 and 200Hz.

4.1. Illustration for Theorem 3.1. We compare the Ritz values of $(A + 10B)^{-1}B$ for Problems 1 and 2 and their residual norms after $k = 10$ Arnoldi/Lanczos steps, started with a random initial vector. Theorem 3.1 states that the Ritz values obtained by B-orthogonalization and standard orthogonalization lie within a distance of $\rho\sqrt{\kappa(B)}$ where ρ is the residual norm (2.4). For Problem 1, we have $h_{k+1,k} = 3.8375 \cdot 10^{-7}$, $t_{k+1,k} = 4.1245 \cdot 10^{-6}$ and $\kappa(W_{k+1}) = 24.755$ and for Problem 2, we have $h_{k+1,k} = 4.1966 \cdot 10^{-7}$, $t_{k+1,k} = 3.2867 \cdot 10^{-7}$ and $\kappa(W_{k+1}) = 2.7$. These values are consistent with Theorem 2.4. The matching significant digits of the respective Ritz values and the residual norms are shown in Tables 4.1 and 4.2, except for the multiple eigenvalue at 0.1 ($\theta_1, \ldots, \theta_4$) for Problem 1, which is not displayed. Ritz values that do not share any digits are not shown. All Ritz values satisfy Theorem 2.5.

4.2. Illustration of the B-orthogonalization of the 'Ritz' vectors. When Ritz vectors are computed by Arnoldi's method with standard orthogonalization, they are not B-orthogonal. We could perform an explicit B-orthogonal projection by solving (3.5). Instead, we use the columns of Y_l as Ritz vectors, as suggested in §3. We illustrate Theorem 3.2, which states that the columns of Y_l are sufficiently accurate Ritz vectors. The θ_j are unchanged. The results reported come from the Arnoldi computations from §4.1. The 'Ritz' vectors before and after B-orthogonalization are denoted by x_j and y_j respectively. Tables 4.3 and 4.4 show the explicitly computed residual norms before and after B-orthogonalization. (Note that the $\rho_j^{(2)}$ in Tables 4.3 and 4.4 corresponds well to the ρ_j in Tables 4.1 and 4.2 respectively. The difference is that ρ_j is computed from (2.4) and $\rho_j^{(2)}$ is the explicitly computed residual norm.)

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TABLE 4.1
Matching the eigenvalues of H_k and T_k after 10 steps for Problem 1. The value ρ_j is defined by (2.4).

j		$\langle x, y\rangle = x^T y$	$\langle x, y\rangle = x^T By$
	θ_j	ρ_j	ρ_j
5	$5.941 \cdot 10^{-6}$	$7 \cdot 10^{-9}$	$4 \cdot 10^{-9}$
6	$3.98875 \cdot 10^{-6}$	$5 \cdot 10^{-8}$	$4 \cdot 10^{-8}$
7	$1 \cdot 10^{-6}$	$9 \cdot 10^{-7}$	$6 \cdot 10^{-7}$
8	$8 \cdot 10^{-7}$	$2 \cdot 10^{-7}$	$2 \cdot 10^{-7}$
9		$2 \cdot 10^{-7}$	$3 \cdot 10^{-7}$
10		$1 \cdot 10^{-7}$	$2 \cdot 10^{-8}$

TABLE 4.2
Matching the eigenvalues of H_k and T_k after 10 steps for Problem 2. The value ρ_j is defined by (2.4).

j		$\langle x, y\rangle = x^T y$	$\langle x, y\rangle = x^T By$
	θ_j	ρ_j	ρ_j
1	$9.9999999994941 \cdot 10^{-2}$	$0.$	$0.$
2	$6.260362 \cdot 10^{-6}$	$2 \cdot 10^{-13}$	$2 \cdot 10^{-13}$
3	$2.208 \cdot 10^{-6}$	$2 \cdot 10^{-9}$	$2 \cdot 10^{-9}$
4	$1.8 \cdot 10^{-6}$	$2 \cdot 10^{-7}$	$2 \cdot 10^{-7}$
5	$1.364 \cdot 10^{-6}$	$3 \cdot 10^{-8}$	$3 \cdot 10^{-8}$
6	$8 \cdot 10^{-7}$	$2 \cdot 10^{-7}$	$3 \cdot 10^{-7}$
7	$6 \cdot 10^{-7}$	$3 \cdot 10^{-7}$	$2 \cdot 10^{-7}$
8	$2 \cdot 10^{-7}$	$1 \cdot 10^{-7}$	$1 \cdot 10^{-7}$
9		$7 \cdot 10^{-8}$	$8 \cdot 10^{-8}$
10		$2 \cdot 10^{-8}$	$2 \cdot 10^{-8}$

The results are consistent with Theorem 3.2. In Table 4.3, $\rho_4^{(B)} \approx 10^{-6}$, which is much larger than $\rho_4^{(2)}$. This is possible since y_4 is a linear combination of $x_1, \ldots, x_4$ and $\rho_4^{(B)}$ depends on $\|R_4\| \approx \rho_1^{(2)} \approx 10^{-5}$.

4.3. Illustration for the implicitly restarted Arnoldi/Lanczos methods. In practical calculations, if small residual norms need to be obtained for the desired eigenvalues, the Krylov subspaces often become very large. In the literature, some remedies against the growth of this subspace are proposed. One idea is to restart the Krylov method with a new pole σ in (1.4), as suggested in [10, 7]. In this paper, we use the implicitly restarted Lanczos and Arnoldi methods with exact shifts [21, 11]. Roughly speaking, the implicitly restarted Arnoldi method is mathematically equivalent to the following scheme.

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TABLE 4.3
Residual norms for Problem 1 before and after B-orthogonalization. We denote $\rho_j^{(2)} = \|(A+10B)^{-1}Bx_j - \theta_j x_j\|$ *and* $\rho_j^{(B)} = \|(A+10B)^{-1}By_j - \theta_j y_j\|_B$.

j	$\rho_j^{(2)}$	$\rho_j^{(B)}$
1	$3{\cdot}10^{-5}$	$5{\cdot}10^{-6}$
2	$6{\cdot}10^{-9}$	$8{\cdot}10^{-7}$
3	$2{\cdot}10^{-8}$	$2{\cdot}10^{-6}$
4	$9{\cdot}10^{-9}$	$2{\cdot}10^{-6}$
5	$7{\cdot}10^{-9}$	$1{\cdot}10^{-7}$
6	$5{\cdot}10^{-8}$	$1{\cdot}10^{-7}$
7	$9{\cdot}10^{-7}$	$3{\cdot}10^{-6}$
8	$2{\cdot}10^{-7}$	$8{\cdot}10^{-7}$
9	$2{\cdot}10^{-7}$	$3{\cdot}10^{-6}$
10	$1{\cdot}10^{-7}$	$4{\cdot}10^{-8}$

TABLE 4.4
Residual norms for Problem 2 before and after B-orthogonalization. We denote $\rho_j^{(2)} = \|(A+10B)^{-1}Bx_j - \theta_j x_j\|$ *and* $\rho_j^{(B)} = \|(A+10B)^{-1}By_j - \theta_j y_j\|_B$.

j	$\rho_j^{(2)}$	$\rho_j^{(B)}$
1	$6{\cdot}10^{-17}$	$4{\cdot}10^{-17}$
2	$4{\cdot}10^{-13}$	$4{\cdot}10^{-13}$
3	$6{\cdot}10^{-9}$	$5{\cdot}10^{-9}$
4	$3{\cdot}10^{-8}$	$3{\cdot}10^{-8}$
5	$1{\cdot}10^{-7}$	$1{\cdot}10^{-7}$
6	$2{\cdot}10^{-7}$	$2{\cdot}10^{-7}$
7	$2{\cdot}10^{-7}$	$2{\cdot}10^{-7}$
8	$1{\cdot}10^{-7}$	$1{\cdot}10^{-7}$
9	$6{\cdot}10^{-8}$	$1{\cdot}10^{-7}$
10	$2{\cdot}10^{-8}$	$9{\cdot}10^{-8}$

ALGORITHM 2. *(implicitly) restarted Arnoldi method*

0. Given is an initial vector v_1.
1. **Iterate :**
   1.1. Form V_{k+1} and $\underline{H}_k$ by k steps of Arnoldi.
   1.2. Compute 'Ritz' pairs (θ, x) and residual norm ρ.
   1.3. Get a new initial vector $v_1 = V_k z$.
   Until $\rho \leq \text{TOL}|\theta|$

The implicitly restarted Arnoldi method is an efficient and reliable implementation of this algorithm. For the problems that are solved in this paper, the new initial vector v_1 is a linear combination of the wanted 'Ritz' vectors, so that 'unwanted' eigenvalues do not show up in following iterations. (For a precise definition and practical algorithms, see [21, 11].) In general, the implicitly restarted Arnoldi and Lanczos methods do not have the same subspaces after two iterations, since the 'Ritz' vectors are different and so is the linear combination. This can lead to different subspaces and therefore to different rates of convergence. The numerical results are obtained using the ARPACK routines `dsaupd` (Lanczos) and `dnaupd` (Arnoldi) [13]. Note that ARPACK uses the Arnoldi process, i.e., full (re)orthogonalization,

TABLE 4.5
Comparison between implicitly restarted Lanczos ($x^T By$) and Arnoldi ($x^T y$) for Problem 3

$\langle x, y\rangle$	linear solves	matrix vector products with B	iterations	time (sec.)
$x^T By$	46	136	4	150.
$x^T y$	46	65	4	117.

TABLE 4.6
Comparison between implicitly restarted Lanczos ($x^T By$) and Arnoldi ($x^T y$) for Problem 4

$\langle x, y\rangle$	linear solves	matrix vector products with B	iterations	time (sec.)
$x^T By$	27	75	2	705
$x^T y$	26	37	2	685

for symmetric problems, rather than the more efficient Lanczos process with partial reorthogonalization. This implies that timings reductions are possible for the results of the Lanczos method with B-orthogonalization. The matrix B was represented by a compressed sparse row matrix storage format, which allows for efficient storage and matrix vector products. The linear system solvers where solved by a block skyline (or profile) solver. All computations were carried out within the SYSNOISE [22] environment on an HP PA 7100 C110 workstation.

Table 4.5 contains the numerical results for Problem 3. The 20 eigenmodes nearest 0 are required. The Implicitly Restarted Arnoldi/Lanczos methods were run with the same initial vector, Krylov subspace dimension $k = 30$, and relative residual tolerance $\text{TOL} = 10^{-5}$. The number of iterations are equal for both methods. The Lanczos method with B-orthogonalization is more expensive due to the additional matrix vector products in the reorthogonalization of the B-orthogonalization. For the Arnoldi method with standard orthogonalization, the number of matrix vector products with B is equal to the number of solves with $A - \sigma B$ plus the number needed for the B-orthogonalization of the Ritz vectors (§3).

Table 4.6 contains the numerical results for Problem 4. The eigenfrequencies between 0 and 250 Hz are sought. The implicitly restarted Arnoldi/Lanczos methods were run with the same initial vector, Krylov subspace dimension $k = 21$, and relative residual tolerance $\text{TOL} = 10^{-5}$. A matrix vector product by B is cheap compared to a back transformation. The conclusions are very similar to Problem 3, but the differences between the CPU times are less pronounced.

5. Extension to (Navier) Stokes problems. Recall the (Navier) Stokes problem (1.3). For this problem, B is typically positive semi-definite. The use of the B-*semi*-inner product in the Lanczos method was suggested by Ericsson [5], Nour-Omid, Parlett, Ericsson and Jensen [5]. The use of this semi-inner product was justified by Ericsson [5] and Meerbergen and Spence [16]. Moreover, it 'purifies' the Ritz values from possible contamination arising from the singularity of B. For the details, see [5, 18, 16]. Cliffe, Garratt, Golding and Spence [2] suggested the use of the matrix

$$P = \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} \qquad \text{instead of} \qquad \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}$$

in the inner product. This P-inner product has the same 'purification' property as the B-inner product (see [16, Theorem 2] with $M = I$). Thus, an alternative to the Arnoldi method with

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B-orthogonalization is the Arnoldi method with P-orthogonalization. In fact, the situation is very similar to acoustic and structural eigenvalue problems. Indeed, decompose

$$V_{k+1} = \begin{bmatrix} U_{k+1} \\ Q_{k+1} \end{bmatrix} \qquad \text{and} \qquad W_{k+1} = \begin{bmatrix} \tilde{U}_{k+1} \\ \tilde{Q}_{k+1} \end{bmatrix}$$

and normalize V_{k+1} such that $V_{k+1}^T P V_{k+1} = U_{k+1}^T U_{k+1} = I$ and W_{k+1} such that $W_{k+1}^T B W_{k+1} = \tilde{U}_{k+1}^T M \tilde{U}_{k+1} = I$. Consequently, Theorem 2.4 is still valid with the only difference that $\kappa(B)$ should be replaced by $\kappa(M)$, V_{k+1} by U_{k+1} and W_{k+1} by $\tilde{U}_{k+1}$.

6. Conclusions and final remarks. In this paper, we established a theoretical comparison between standard orthogonalization and B-orthogonalization for the solution of eigenvalue problems, for which the square root of the condition number of the mass matrix is small. This is often the case in acoustic and structural eigenvalue problems and for the discretized (Navier) Stokes equations. Roughly speaking, the orthogonalization seems to play a minor role in the convergence of the eigenvectors in the Krylov space. The theoretical results are extended to the Navier-Stokes problem as well, where the Arnoldi method with B-semi-orthogonalization and the Arnoldi method with P-semi-orthogonalization behave similarly.

Following the theory and our numerical experiments the type of inner product should not be chosen on the basis of rates of convergence. The decision should be based on cost per iteration, or reliability. For example, it follows from the numerical results for Problem 4 that there is no advantage in performance for the Arnoldi method with standard orthogonalization with respect to the Lanczos method with B-orthogonalization, though the inner product is more expensive for the Lanczos method. Moreover, when the number of iteration vectors is high, it is expected that the Gram-Schmidt process with reorthogonalization becomes prohibitive, so that the Lanczos method becomes much cheaper than the Arnoldi method. We also noticed that the Lanczos method with B-orthogonalization is more reliable than the Arnoldi method with standard orthogonalization: sometimes, sought-after eigenvalues are missed by the Arnoldi method. For Navier-Stokes applications, where the Arnoldi method should be used anyway since A is nonsymmetric, the use of the P-inner product rather than the B-inner product may lead to a more efficient code. Lehoucq and Scott [12] report that the B-inner product seems to be more reliable than the standard inner product. They do not report results for the P-inner product.

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