Generalized Davidson and multidirectional-type methods for the generalized singular value decomposition

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Abstract. We propose new iterative methods for computing nontrivial extremal generalized singular values and vectors. The first method is a generalized Davidson-type algorithm and the second method employs a multidirectional subspace expansion technique. Essential to the latter is a fast truncation step designed to remove a low quality search direction and to ensure moderate growth of the search space. Both methods rely on thick restarts and may be combined with two different deflation approaches. We argue that the methods have monotonic and (asymptotic) linear convergence, derive and discuss locally optimal expansion vectors, and explain why the fast truncation step ideally removes search directions orthogonal to the desired generalized singular vector. Furthermore, we identify the relation between our generalized Davidson-type algorithm and the Jacobi–Davidson algorithm for the generalized singular value decomposition. Finally, we generalize several known convergence results for the Hermitian eigenvalue problem to the Hermitian positive definite generalized eigenvalue problem. Numerical experiments indicate that both methods are competitive.

Key words. Generalized singular value decomposition, GSVD, generalized singular value, generalized singular vector, generalized Davidson, multidirectional subspace expansion, subspace truncation, thick restart.

AMS subject classification. 15A18, 15A23, 15A29, 65F15, 65F22, 65F30, 65F50.

1 Introduction

The generalized singular value decomposition (GSVD) [17] is a generalization of the standard singular value decomposition (SVD), and is used in, for example, linear discriminant analysis [10], the method of particular solutions [3], general form Tikhonov regularization [6, Sec. 5.1], and more [1]. Computing the full GSVD with direct methods can be prohibitively time-consuming for large problem sizes; however, for many applications it suffices to compute only a few of the largest or smallest generalized singular values and vectors. As a result, iterative methods may become attractive when the matrices involved are large and sparse.

An early iterative approach based on a modified Lanczos method was introduced by Zha [23], and later a variation by Kilmer, Hansen, and Español [11]. Both methods are inner-outer methods that require the solution to a least squares problem in each iteration, which may be computationally expensive. An approach that naturally allows for inexact solutions is the Jacobi–Davidson-type method (JDGSVD) introduced in [8]; however, this is still an inner-outer method. Alternatives to the previously mentioned methods include iterative methods designed for (symmetric positive definite) generalized eigenvalue problems, in particular generalized Davidson [12, 14] and LOBPCG [13]. These methods compute only the right generalized singular vectors and require additional steps to determine the left generalized singular vectors. More importantly, applying these methods involves squaring potentially ill-conditioned matrices.

In this paper we discuss two new and competitive iterative methods for the computation of extremal generalized singular values and corresponding generalized singular vectors. The first can be

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We generalize several known error bounds for the Hermitian eigenvalue problem to results for the GSVD. A crucial part of both methods is a thick restart that allows for the removal of unwanted elements. Triangular and diagonal are two closely related forms of the GSVD. The triangular form is practical and can be partitioned as

\[ AW = UΣ_AR \quad \text{and} \quad BW = VΣ_BR. \]

The remainder of this text is organized as follows. We derive a generalized Davidson-type algorithm for the GSVD in the next section, and prove multiple related theoretical properties. We subsequently discuss a B-B orthonormal version of the algorithm and its connection to JDGSVD in Section 3. In Section 4, we examine locally optimal search directions and argue for a multidirectional subspace expansion followed by a fast subspace truncation; then we present our second algorithm. In Section 5, we explore the deflation of generalized singular values and generalized singular vectors. We generalize several known error bounds for the Hermitian eigenvalue problem to results for the generalized singular value decomposition in Section 6. Finally, we consider numerical examples and experiments in Section 7, and end with conclusions in Section 8.

2 Generalized Davidson for the GSVD

Triangular and diagonal are two closely related forms of the GSVD. The triangular form is practical for the derivation and implementation of our methods, while the diagonal form is particularly relevant for the analysis. We adopt the definitions from Bai [1], but with a slightly more compact presentation. Let \( A \) be an \( m \times n \) matrix, \( B \) a \( p \times n \) matrix, and assume for the sake of simplicity that \( \mathcal{N}(A) \cap \mathcal{N}(B) = \{0\} \); then \( \text{rank}([A^TB^T]^T) = n \) and there exist unitary matrices \( U, V, W \), an \( m \times n \) matrix \( Σ_A \), a \( p \times n \) matrix \( Σ_B \), and a nonsingular upper-triangular \( n \times n \) matrix \( R \) such that

\[ (1) \quad AW = UΣ_AR \quad \text{and} \quad BW = VΣ_BR. \]

The matrices \( Σ_A \) and \( Σ_B \) satisfy

\[ Σ_A^TΣ_A = \text{diag}(c_1^2, \ldots, c_m^2), \quad Σ_B^TΣ_B = \text{diag}(s_1^2, \ldots, s_n^2), \quad Σ_A^TΣ_A + Σ_B^TΣ_B = I, \]

and can be partitioned as

\[
\begin{bmatrix}
D_A & 0 & 0 \\
0 & I & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

\[
\begin{bmatrix}
D_B & 0 & 0 \\
0 & 0 & I \\
0 & 0 & 0
\end{bmatrix}
\]

where \( l = \min\{m, p, n, m + p - n\} \), \( (\cdot)_+ = \max\{\cdot, 0\} \), and \( D_A \) and \( D_B \) are diagonal matrices with nonnegative entries. The generalized singular pairs \((c_j, s_j)\) are nonnegative and define the regular generalized singular values \( σ_j = \infty \) if \( s_j = 0 \) and \( σ_j = c_j/s_j \) otherwise. Hence, we call a generalized singular pair \((c_j, s_j)\) large if \( σ_j \) is large and small if \( σ_j \) is small, and additionally refer to the largest and smallest \( σ_j \) as \( σ_{\max} \) and \( σ_{\min} \), respectively. The diagonal counterpart of (1) is

\[ (2) \quad AX = UΣ_A \quad \text{and} \quad BX = VΣ_B \quad \text{with} \quad X = WR^{-1}, \]

and is useful because the columns of \( X \) are the (right) singular vectors \( x_j \) and satisfy, for instance,

\[ (3) \quad s_j^2A^∗Ax_j = c_j^2B^∗Bx_j. \]
The assumption \( \mathcal{N}(A) \cap \mathcal{N}(B) = \{0\} \) is not necessary for the implementation of our algorithm; nevertheless, we will make this assumption for the remainder of the text to simplify our discussion and analysis. We may also assume without loss of generality that the desired generalized singular values are contained in the leading principal submatrices of the factors. Consequently, if \( k < l \) and \( C_k, S_k, \) and \( R_k \) denote the leading \( k \times k \) principal submatrices of \( \Sigma_A, \Sigma_B, \) and \( R; \) and \( U_k, V_k, W_k, \) and \( X_k \) denote the first \( k \) columns of \( U, V, W, \) and \( X; \) then \( X_k = W_k R_k^{-1} \) and we can define the partial (or truncated) GSVD of \( (A, B) \) as

\[
AW_k = U_k C_k R_k \quad \text{and} \quad BW_k = V_k S_k R_k.
\]

We aim is to approximate this partial GSVD for a \( k \ll n. \)

Since (3) can be interpreted as a generalized eigenvalue problem, it appears reasonable to consider the search space

\[
\mathcal{W}_k = \text{span}\{\tilde{x}_0, (s^2(0) A^T A - \tilde{c}_0^2 B^T B) \tilde{x}_0, (s^2(1) A^T A - \tilde{c}_1^2 B^T B) \tilde{x}_1, \ldots, (s^2(k-1) A^T A - \tilde{c}_{k-1}^2 B^T B) \tilde{x}_{k-1}\},
\]

consisting of homogeneous residuals generated by the generalized Davidson method (c.f., e.g., [14, Sec. 11.2.4] and [12, Sec. 11.3.6]) applied to the matrix pencil \((A^T A, B^T B)\). The quantities \( \tilde{x}_j, \tilde{c}_j, \) and \( \tilde{s}_j \) are approximations to \( x_j, c_j, \) and \( s_j \) with respect to the search space \( \mathcal{W}_j \). The challenge is to compute a basis \( \mathcal{W}_k \) with orthonormal columns for \( \mathcal{W}_k \) without using the products \( A^T A \) and \( B^T B \); however, let us focus on the extraction phase first. We will later see that a natural subspace expansion follows as a consequence.

Given \( W_k, \) we can compute the reduced QR decompositions

\[
(4) \quad AW_k = U_k H_k, \quad BW_k = V_k K_k,
\]

where \( U_k \) and \( V_k \) have \( k \) orthonormal columns and \( H_k \) and \( K_k \) are \( k \times k \) and upper-triangular. To compute the approximate generalized singular values, let the triangular form GSVD of \((H_k, K_k)\) be given by

\[
H_k \tilde{W} = \tilde{U} \tilde{C} \tilde{R}, \quad K_k \tilde{W} = \tilde{V} \tilde{S} \tilde{R},
\]

where \( \tilde{U}, \tilde{V}, \) and \( \tilde{W} \) are orthonormal, \( C \) and \( S \) are diagonal, and \( R \) is upper triangular. At this point, we can readily form the approximate partial GSVD

\[
(5) \quad A(W_k \tilde{W}) = (U_k \tilde{U}) \tilde{C} \tilde{R}, \quad B(W_k \tilde{W}) = (V_k \tilde{V}) \tilde{S} \tilde{R},
\]

and determine the leading approximate generalized singular values and vectors. When the dimension of the search space \( \mathcal{W}_k \) grows large, a thick restart can be performed by partitioning the decompositions in (5) as

\[
(6) \quad A \begin{bmatrix} W_k \tilde{W}_1 & W_k \tilde{W}_2 \end{bmatrix} = \begin{bmatrix} U_k \tilde{U}_1 & U_k \tilde{U}_2 \end{bmatrix} \begin{bmatrix} \tilde{C}_1 & \tilde{C}_2 \\ \tilde{C}_1 & \tilde{C}_2 \end{bmatrix} \begin{bmatrix} \tilde{R}_{11} & \tilde{R}_{12} \\ \tilde{R}_{21} & \tilde{R}_{22} \end{bmatrix},
\]

\[
B \begin{bmatrix} W_k \tilde{W}_1 & W_k \tilde{W}_2 \end{bmatrix} = \begin{bmatrix} V_k \tilde{V}_1 & V_k \tilde{V}_2 \end{bmatrix} \begin{bmatrix} \tilde{S}_1 & \tilde{S}_2 \\ \tilde{S}_1 & \tilde{S}_2 \end{bmatrix} \begin{bmatrix} \tilde{R}_{11} & \tilde{R}_{12} \\ \tilde{R}_{21} & \tilde{R}_{22} \end{bmatrix},
\]

and truncating to

\[
A(W_k \tilde{W}_1) = (U_k \tilde{U}_1) \tilde{C}_1 \tilde{R}_{11}, \quad B(W_k \tilde{W}_1) = (V_k \tilde{V}_1) \tilde{S}_1 \tilde{R}_{11}.
\]
If there is need to reorder the $c_j$ and $s_j$, then we can simply use the appropriate permutation matrix $P$ and compute

\[
A(W_k \tilde{W}Q) = (U_k \tilde{U}P)(P^*CP)(P^*RQ),
B(W_k \tilde{W}Q) = (V_k \tilde{V}P)(P^*SP)(P^*RQ),
\]

where $Q$ is unitary and such that $P^*RQ$ is upper triangular.

For a subsequent generalized Davidson-type expansion of the search space, let

\[
\begin{align*}
\tilde{u}_1 &= U_1 \tilde{U}_1 e_1, & \tilde{v}_1 &= V_1 \tilde{V}_1 e_1, & \tilde{w}_1 &= W_1 \tilde{W}_1 e_1, & \text{and } \tilde{x}_1 &= \tilde{w}_1 / r_{11}
\end{align*}
\]

be the approximate generalized singular vectors satisfying

\[
A\tilde{x}_1 = \tilde{c}_1 \tilde{u}_1 \quad \text{and} \quad B\tilde{x}_1 = \tilde{s}_1 \tilde{v}_1.
\]

Then the homogeneous residual given by

\[
(7) \quad r = (\tilde{s}_1^2 A^*A - \tilde{c}_1^2 B^*B)\tilde{x}_1 = \tilde{c}_1 \tilde{s}_1 (\tilde{s}_1 A^*\tilde{u}_1 - \tilde{c}_1 B^*\tilde{v}_1)
\]

suggests the expansion vector $\tilde{r} = \tilde{s}_1 A^*\tilde{u}_1 - \tilde{c}_1 B^*\tilde{v}_1$, which is orthogonal to $W_k$. The residual norm $\|r\|$ goes to zero as the generalized singular value and vector approximations converge, and we recommend terminating the iterations when the right-hand side of

\[
(8) \quad \frac{\|r\|}{(\tilde{s}_1^2 \|A^*A\| + \tilde{c}_1^2 \|B^*B\|) \|\tilde{x}_1\|} \leq \frac{\sqrt{n} \|r_{11}\| \|r\|}{\tilde{s}_1 \|A^*A\|_1 + \tilde{c}_1 \|B^*B\|_1}
\]

is sufficiently small. The left-hand side is the normwise backward error by Tisseur [21], and the right-hand side is an alternative that can be approximated efficiently; for example, using the normest1 function in MATLAB, which does not require computing the matrix products $A^*A$ and $B^*B$ explicitly. The GDGSVD algorithm is summarized in Algorithm 1.

**Algorithm 1** (Generalized Davidson for the GSVD (GDGSVD)).

**Input:** Matrix pair $(A, B)$, starting vector $w_0$, minimum and maximum dimensions $j < \ell$.

**Output:** $AW_j = U_j C_j R_j$ and $BW_j = V_j S_j R_j$ approximating a partial GSVD.

1. Let $\tilde{r} = w_0$.
2. for number of restarts and not converged (cf., e.g., (8)) do
   3. for $k = 1, 2, \ldots, \ell$ do
      4. $w_k = \tilde{r} / \|\tilde{r}\|$.
      5. Update $AW_k = U_k H_k$ and $BW_k = V_k K_k$.
      6. Compute $H_k = \tilde{U} \tilde{C} \tilde{R} \tilde{W}^*$ and $K_k = \tilde{V} \tilde{S} \tilde{R} \tilde{W}^*$.
      7. Let $\tilde{r} = s_1 A^*\tilde{u}_1 - c_1 B^*\tilde{v}_1$.
      8. if $j \leq k$ and converged (cf., e.g., (8)) then break
   9. end
10. Partition $\tilde{U}, \tilde{V}, \tilde{W}, \tilde{C}, \tilde{S},$ and $\tilde{R}$ according to (6).
11. Let $U_j = U_k \tilde{U}_1, V_j = V_k \tilde{V}_1, \text{and } W_j = W_k \tilde{W}_1$.
12. Let $H_j = \tilde{C}_1 \tilde{R}_{11}$ and $K_j = \tilde{S}_1 \tilde{R}_{11}$.
13. end

By design, the largest (or smallest) Ritz values are preserved after the restart; moreover, the generalized singular values increase (or decrease) monotonically per iteration as indicated by the proposition below. We wish to emphasize that the proof of the proposition does not require $B^*B$ to be nonsingular, as opposed to the Courant–Fischer minimax principles for the generalized eigenvalue problem.
**Proposition 1.** Let $\mathcal{W}_k$ and $\mathcal{W}_{k+1}$ be subspaces of dimensions $k$ and $k + 1$, respectively, and such that $\mathcal{W}_k \subset \mathcal{W}_{k+1}$. If $\sigma_{\max}(\mathcal{W})$ and $\sigma_{\min}(\mathcal{W})$ denote the maximum and minimum generalized singular values of $A$ and $B$ with respect to the subspace $\mathcal{W}$, then

$$\sigma_{\max} \geq \sigma_{\max}(\mathcal{W}_{k+1}) \geq \sigma_{\max}(\mathcal{W}_k) \geq \sigma_{\min}(\mathcal{W}_k) \geq \sigma_{\min}(\mathcal{W}_{k+1}) \geq \sigma_{\min}.$$ 

**Proof.** Both $A^*A$ and $B^*B$ may be singular; therefore, we consider the pencil

$$(A^*A, A^*A + B^*B) = (A^*A, X^*X^{-1})$$

with generalized eigenvalues $c_i^2$ and note that $\sigma_i^2 = c_i^2/(1 - c_i^2)$ with the convention that $1/0 = \infty$. Applying the Courant–Fischer minimax principles yields

$$c_1 \geq \max_{0 \neq w \in \mathcal{W}_k} \frac{||Aw||}{||X^{-1}w||} \geq \max_{0 \neq w \in \mathcal{W}_k} \frac{||Aw||}{||X^{-1}w||} \geq \min_{0 \neq w \in \mathcal{W}_k} \frac{||Aw||}{||X^{-1}w||} \geq \min_{0 \neq w \in \mathcal{W}_{k+1}} \frac{||Aw||}{||X^{-1}w||} \geq c_n.$$ 

\[\square\]

**Proposition 1** implies that if a basis $W_k$ for a subspace $\mathcal{W}_k$ is computed by Algorithm 1, then

$$\sigma_{\max}(\mathcal{W}_k) = \max_{0 \neq w \in \mathcal{W}_k} \frac{||Aw||}{||X^{-1}w||} = \max_{c \in \mathbb{C}} \frac{||AW_kc||}{||X^{-1}w||} = \max_{c \in \mathbb{C}} \frac{||AW_kc||}{||X^{-1}w||} \geq \frac{||H_kc||}{||X^{-1}w||},$$

that is, the largest generalized singular value of the matrix pair $(A, B)$ with respect to the subspace $\mathcal{W}_k$ is the largest generalized singular value of $(H_k, K_k)$. A similar statement holds for the smallest generalized singular value. Furthermore, the matrix pair $(H_k, K_k)$ is optimal in the sense of the following proposition.

**Proposition 2.** Let the $M$-Frobenius norm for a Hermitian positive definite matrix $M$ be defined as $||Y||_{F,M}^2 = \text{trace}(Y^*MY)$. Now consider the decompositions from (4) and define the residuals

- $R_1(G) = AW_k - U_kG$,
- $R_2(G) = BW_k - V_kG$,
- $R_3(G) = A^*U_k - B^*V_kG^*$,
- $R_4(G) = B^*V_k - A^*U_kG^*$;

then the following results hold.

1. $G = H_k = U_k^*AW_k$ minimizes $||R_1(G)||_2$ and is the unique minimizer of $||R_1(H_k)||_F$.
2. $G = K_k = V_k^*BW_k$ minimizes $||R_2(G)||_2$ and is the unique minimizer of $||R_2(K_k)||_F$.
3. If $B^*B$ is nonsingular, then $G = H_kK_k^{-1}$ minimizes $||R_3(G)||_{(B^*B)^{-1}}$ and is the unique minimizer of $R_3$ with respect to the $(B^*B)^{-1}$-Frobenius norm.
4. If $A^*A$ is nonsingular, then $G = K_kH_k^{-1}$ minimizes $||R_4(G)||_{(A^*A)^{-1}}$ and is the unique minimizer of $R_4$ with respect to the $(A^*A)^{-1}$-Frobenius norm.

**Proof.** With the observation that $A^*U_k = A^*AW_kH_k^{-1}$ and $B^*V_k = B^*BW_kK_k^{-1}$, the proof becomes a straightforward adaptation of [8, Thm 2.1]. \[\square\]

Propositions 1 and 2 demonstrate that the convergence behavior of Algorithm 1 is monotonic, and that the computed $H_k$ and $K_k$ are in some sense optimal for the search space $\mathcal{W}_k = \text{span}(W_k)$; however, the propositions make no statement regarding the quality of the subspace expansion. A locally optimal residual-type subspace expansion can be derived with inspiration from Ye [22].
Proposition 3. Define

\[ R_k = A^* W_k (H_k^* H_k + K_k^* K_k)^{-1} K_k^* K_k - B^* B W_k (H_k^* H_k + K_k^* K_k)^{-1} H_k^* H_k \]

and let \( r = R_k c \); then

\[ \cos^2(x_1, [W_k r]) = \cos^2(x_1, W_k) + \cos^2(x_1, r) \]

is maximized for \( c = R_k^+ x_1 \).

**Proof.** Since \( N(A) \cap N(B) = \{0\} \) we also have \( N(H_k) \cap N(K_k) = \{0\} \), which implies that \( H_k^* H_k + K_k^* K_k \) is invertible and \( R_k \) is well-defined. Furthermore, it is now straightforward to verify that

\[ W_k^* R_k = H_k^* H_k (K_k^* K_k)^{-1} K_k^* K_k - K_k^* K_k (H_k^* H_k + K_k^* K_k)^{-1} H_k^* H_k = 0 \]

using the GSVD of \( H_k \) and \( K_k \). It follows that

\[ ||[W_k r]^* x_1||^2 = ||W_k^* x_1||^2 + |r^* x_1|^2, \]

which realizes its maximum for \( c = R_k^+ x_1 \). \( \square \)

Different choices for \( R_k \) in Proposition 3 are possible; however, the current choice does not require additional assumptions on, for instance, \( H_k \) and \( K_k \). Regardless of the choice of \( R_k \), computing the optimal expansion vector is generally impossible without a priori knowledge of the desired generalized singular vector \( x_1 \). Therefore, we expand the search space with a residual-type vector similar to generalized Davidson. The convergence of generalized Davidson is closely connected to steepest descent and has been studied extensively; see, for example, Ovtchinnikov [15, 16] and references therein. For completeness, we add the following asymptotic bound for the GSVD.

Proposition 4. Let \((c_1, s_1)\) be the smallest generalized singular pair of \((A, B)\) with corresponding generalized singular vector \( x_1 \), and assume the pair is simple. Define the Hermitian positive definite operator \( M = s_1^2 A^* A - c_1^2 B^* B \) restricted to the domain perpendicular to \((A^* A + B^* B) x_1 = X^* e_1 \), and let the eigenvalues of \( M \) be given by

\[ \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} > 0. \]

Furthermore, let \( \overline{x}_1, \overline{c}_1 = ||A \overline{x}_1||, \) and \( \overline{s}_1 = ||B \overline{x}_1|| \) approximate \( x_1, c_1, \) and \( s_1 \), respectively, and be such that \( \overline{c}_1^2 + \overline{s}_1^2 = 1 \). If \( \overline{x}_1 = \xi x_1 + f \) for some scalar \( \xi \) and vector \( f \perp X^* e_1 \); then

\[ \sin^2([\overline{x}_1 r], x_1) \leq \left( \frac{\kappa - 1}{\kappa + 1} \right)^2 \sin^2(\overline{x}_1, x_1) + O(||f||^3), \]

where \( \kappa = \lambda_1/\lambda_{n-1} \) is the condition number of \( M \), and \( r = (\overline{s}_1^2 A^* A - \overline{c}_1^2 B^* B) \overline{x}_1 \) is the homogeneous residual.

**Proof.** We have

\[ \overline{c}_1^2 = \overline{x}_1^* A^* A \overline{x}_1 = \xi^2 c_1^2 + ||Af||^2 \quad \text{and} \quad \overline{s}_1^2 = \overline{x}_1^* B^* B \overline{x}_1 = \xi^2 s_1^2 + ||Bf||^2, \]

and it follows that

\[ r = \xi^2 (s_1^2 A^* A - c_1^2 B^* B) f + (||Bf||^2 A^* A - ||Af||^2 B^* B)(\xi x_1 + f) = \xi^2 M f + O(||f||^2) \]

and

\[ r^* x_1 = \xi f^* (s_1^2 A^* A - c_1^2 B^* B) f = \xi f^* M f. \]
Hence, $x_1 = x_1$ if $\|r\| = 0$ for $x_1$ sufficiently close to $x_1$ and we are done. Otherwise, $r$ is nonzero and perpendicular to $x_1$, so that

$$\sin^2([x_1 \ r], x_1) = 1 - \cos^2(x_1, x_1) - \cos^2(r, x_1) = \left(1 - \frac{\cos^2(r, x_1)}{\sin^2(x_1, x_1)}\right) \sin^2(x_1, x_1).$$

Combining the above expressions, and using the fact that nontrivial orthogonal projectors have unit norm, yields

$$\frac{\cos^2(r, x_1)}{\sin^2(x_1, x_1)} = \frac{|r^*x_1|^2}{\|r\|^2\|(I - x_1x_1^*)x_1\|^2} \geq \frac{|f^*Mf|^2}{\|Mf\|^2\|f\|^2} + \mathcal{O}(\|f\|).$$

Using the Kantorovich inequality (cf., e.g., [4, p. 68]) we obtain

$$\sin^2([x_1 \ r], x_1) \leq \left(1 - \frac{4\lambda_1\lambda_{n-1}}{(\lambda_1 + \lambda_{n-1})^2}\right) \sin^2(x_1, x_1) + \mathcal{O}(\|f\| \sin^2(x_1, x_1))$$

$$= \left(\frac{k-1}{k+1}\right)^2 \sin^2(x_1, x_1) + \mathcal{O}(\|f\| \sin^2(x_1, x_1)).$$

Finally, $x_1^2 + x_1^2 = 1$ implies $\|x_1\| \geq \sigma_{\min}(X)$, so that $\sin(x_1, x) \leq \sigma_{\min}^{-1}(X) \||f|| = \mathcal{O}(\|f\|)$.  

The condition number $\kappa$ from Proposition 4 may be large in practice, in which case the quantity $(\kappa - 1)/(\kappa + 1)$ is close to 1. However, this upper bound may be rather pessimistic and we will see considerably faster convergence during the numerical tests in Section 7.

### 3 $B^*B$-orthonormal GDGSVD

In the previous section we have derived the GDGSVD algorithm for an orthonormal basis of $\mathcal{W}_k$. An alternative is to construct a $B^*B$-orthonormal basis of $\mathcal{W}_k$, which allows us to use the SVD instead of the slower GSVD for the projected problem, as well as reduce the amount of work necessary for a restart. Another benefit is that the $B^*B$-orthonormality reveals the connection between GDGSVD and JDGSVD, a Jacobi–Davidson-type algorithm for the GSVD [8].

The derivation of $B^*B$-orthonormal GDGSVD is similar to the derivation of Algorithm 1. Suppose that $B^*B$ is nonsingular, let $\tilde{W}_k$ be a basis of $\mathcal{W}_k$ satisfying $\tilde{W}_k^*B^*B\tilde{W}_k = I$, and compute the QR-decomposition

$$(9) \quad \tilde{A}\tilde{W}_k = \tilde{U}_k\tilde{H}_k,$$

where $\tilde{U}$ has orthonormal columns and $\tilde{H}_k$ is upper-triangular. Note that (9) can be obtained from the QR-decompositions in (4) by setting $\tilde{W}_k = W_kK_k^{-1}, \tilde{U}_k = U_k$, and $\tilde{H}_k = H_kK_k^{-1}$. If $\tilde{H}_k = \tilde{U}\Sigma\tilde{W}^*$ is the SVD of $\tilde{H}_k$; then

$$A(\tilde{W}_k\tilde{W}) = (\tilde{U}_k\tilde{U})\Sigma,$$

which can be partitioned as

$$(10) \quad A \begin{bmatrix} \tilde{W}_k\tilde{W}_1 & \tilde{W}_k\tilde{W}_2 \end{bmatrix} = \begin{bmatrix} \tilde{U}_k\tilde{U}_1 & \tilde{U}_k\tilde{U}_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 \\ \Sigma_2 \end{bmatrix}$$

and truncated to $A\tilde{W}_k\tilde{W}_1 = \tilde{U}_k\tilde{U}_1\Sigma_1$. With $\tilde{u}_1 = \tilde{U}_k\tilde{U}_1\Sigma_1$ and $\tilde{w}_1 = \tilde{W}_k\tilde{W}_1$ we get the residual

$$r = (\tilde{A}\tilde{A} - \sigma_1^2B^*B)\tilde{w}_1 = \sigma_1(\tilde{A}\tilde{u}_1 - \sigma_1B^*B\tilde{w}_1)$$
and the expansion vector \( \vec{\tau} = A\vec{u}_1 - \sigma_1 B^* B\vec{u}_1 \). The expansion vector \( \vec{\tau} \) is orthogonal to \( \vec{W}_k \) in exact arithmetic, but should in practice still be orthogonalized with respect to \( \vec{W}_k \) prior to \( B^*B \)-orthogonalization in order to improve numerical stability and accuracy [7, Sec. 3.5]. Finally, in the \( B^*B \)-orthonormal case the suggested stopping condition (8) becomes

\[
\frac{||r||}{(||A^*A|| + \sigma_1^2||B^*B||)||\vec{w}_1||} \leq \frac{\sqrt{n} ||r||}{(||A^*A||_1 + \sigma_1^2||B^*B||_1)||\vec{w}_1||} \leq \tau
\]

for some tolerance \( \tau \). The algorithm is summarized below in Algorithm 2, where \( \vec{V}_k = B\vec{W}_k \) has orthonormal columns.

**Algorithm 2 (\( B^*B \)-orthonormal GDGSVD).**

**Input:** Matrix pair \((A, B)\), starting vector \( w_0 \), minimum and maximum dimensions \( j < \ell \).

**Output:** Orthonormal \( \vec{U}_j \), \( B^*B \)-orthonormal \( \vec{W}_j \), and diagonal \( \Sigma_j \) satisfying \( A\vec{W}_j = \vec{U}_j\Sigma_j \).

1. Let \( \vec{W}_0 = \vec{V}_0 = [] \) and \( \vec{\tau} = w_0 \).
2. **for** number of restarts and not converged (cf., e.g., (11)) **do**
   3. **for** \( k = 1, 2, \ldots, \ell \) **do**
   4. \( \vec{w}_k = (I - \vec{W}_{k-1})(\vec{W}_{k-1}^*\vec{W}_{k-1})^{-1}\vec{W}_{k-1}^*\vec{r} \).
   5. Compute \( \vec{\tau}_k = B\vec{w}_k \).
   6. \( B^*B \)-orthogonalize: \( \vec{\omega}_k = \vec{w}_k - \vec{W}_{k-1}\vec{\tau}_{k-1} \).
   7. \( \vec{v}_k = (I - \vec{V}_{k-1}\vec{\tau}_{k-1}^*)\vec{v}_{k-1} \).
   8. \( \vec{w}_k = \vec{\omega}_k/||\vec{w}_k|| \) and \( \vec{v}_k = \vec{v}_k/||\vec{v}_k|| \).
   9. Update the QR-decomposition \( A\vec{W}_k = \vec{U}_k\vec{H}_k \).
   10. Compute the SVD \( \vec{H}_k = \vec{U}_k\vec{\Sigma}_k\vec{W}_k^* \).
   11. \( \vec{\tau} = A^*\vec{U}_k\vec{u}_1 - \sigma_1 B^*\vec{V}_k\vec{w}_1 \).
   12. **if** \( j \leq k \) and converged (cf., e.g., (11)) **then** break
   13. **end**
14. Partition \( \vec{U}, \vec{\Sigma} \), and \( \vec{W} \) according to (10).
15. Let \( \vec{U}_j = \vec{U}_k\vec{U}_1, \vec{V}_j = \vec{V}_k\vec{W}_1 \), and \( \vec{W}_j = \vec{W}_k\vec{W}_1 \).
16. Let \( \vec{H}_j = \vec{\Sigma}_1 \).
17. **end**

The product \( B^*B \) may be arbitrarily close to singularity, and a severely ill-conditioned \( B^*B \) may prove to be problematic despite the additional orthogonalization step in Algorithm 2. Therefore, we would generally advise against using Algorithm 2, and recommend using Algorithm 1 and orthonormal bases instead. However, \( B^*B \)-orthonormal GDGSVD relates nicely to JDGSVD on a theoretical level, regardless of the potential practical issues. In JDGSVD the search spaces \( \vec{U}_k \) and \( \vec{W}_k \) are repeatedly updated with the vectors \( s \perp \vec{u}_1 \) and \( t \perp \vec{w}_1 \), which are obtained by solving correction equations. Picking the updates

\[
s = (I - \vec{u}_1\vec{u}_1^*)Ar \quad \text{and} \quad t = r,
\]

instead of solving the correction equations gives JDGSVD the same subspace expansions as \( B^*B \)-orthogonal GDGSVD. Furthermore, standard extraction in JDGSVD is performed by computing the SVD of \( \vec{U}_k^*A\vec{W}_k \), which is identical to the extraction in \( B^*B \)-orthonormal GDGSVD. For harmonic Ritz extraction, JDGSVD uses the harmonic Ritz vectors \( \vec{U}_k c \) and \( \vec{W}_k d \), where \( c \) and \( d \) solve

\[
\vec{W}_k^* A^* A \vec{W}_k \vec{d} = \sigma^2 \vec{W}_k^* B^* B \vec{W}_k \vec{d} \quad \text{and} \quad \vec{c} = \sigma (\vec{W}_k^* A^* \vec{U}_k)^{-1} \vec{W}_k^* B^* B \vec{W}_k \vec{d}.
\]

The above simplifies to

\[
\vec{W} \Sigma^2 \vec{W}^* \vec{d} = \sigma^2 \vec{d} \quad \text{and} \quad \vec{c} = \sigma \vec{U} \Sigma^{-1} \vec{W}^* \vec{d}.
\]
for $B^*B$-orthonormal GDGSVD and produces the same primitive Ritz vectors as the standard extraction. To summarize, JDGSVD coincides with $B^*B$-orthonormal GDGSVD for specific expansion vectors, and there is no difference between standard and harmonic extraction in $B^*B$-orthonormal GDGSVD. The difference in practice between the two methods is primarily caused by the different expansion phases, where GDGSVD uses residual-type vectors and JDGSVD normally solves correction equations. In the next section we will discuss how the subspace expansion for GDGSVD may be further improved.

4 Multidirectional subspace expansion

While the residual vector $r$ from (7) is a practical choice for the subspace expansion, it is not necessarily optimal. In fact, neither is the vector given by Proposition 3, which is only the optimal “residual-type” expansion vector. In their most general form, the desired expansion vectors are

\[(12) \quad a - b, \quad \text{where} \quad a = (I - W_k W_k^*) A^* A W_k c_* \quad \text{and} \quad b = (I - W_k W_k^*) B^* B W_k d_*,\]

for some “optimal” choice of $c_*$ and $d_*$. The following proposition characterizes $c_*$ and $d_*$.

**Proposition 5.** Let $R_k$ and $r$ be defined as in Proposition 3, and assume that $R_k$ has full column rank. If $R_k^* A^* A W_k$ and $R_k^* B^* B W_k$ are nonsingular and if $s = S_k d$ with

\[S_k = (A^* A W_k - W_k H_k^* H_k)(R_k^* A^* A W_k)^{-1} - (B^* B W_k - W_k K_k^* K_k)(R_k^* B^* B W_k)^{-1};\]

then

\[\cos^2(x_1, [W_k r s]) = \cos^2(x_1, W_k) + \cos^2(x_1, r) + \cos^2(x_1, s)\]

is maximized for $c = R_k^* x_1$ and $d = S_k^* x_1$. Moreover, for any $c, d,$ and scalar $t$, the linear combination $R_k c + t S_k d$ can be written in the form of (12). The mapping from $c$ and $d$ to $c_*$ and $d_*$ is one-to-one if $t \neq 0$.

**Proof.** For the first part of the proof, use that $W_k^* R_k = W_k^* S_k = R_k^* S_k = 0$. For the second part, define the shorthand $M = H_k^* H_k + K_k^* K_k$ and recall that

\[R_k = A^* A W_k M^{-1} K_k^* K_k - B^* B W_k M^{-1} H_k^* H_k.\]

Hence, for any $c, d$ and scalar $t$ we have

\[R_k c + t S_k d = (I - W_k W_k^*) R_k c + t (I - W_k W_k^*) S_k d\]
\[= (I - W_k W_k^*) A^* A W_k (M^{-1} K_k^* K_k c + t (R_k^* A^* A W_k)^{-1} d)\]
\[- (I - W_k W_k^*) B^* B W_k (M^{-1} H_k^* H_k c + t (R_k^* B^* B W_k)^{-1} d)\]
\[= a - b,\]

where $a$ and $b$ are defined as in (12) for the $c_*$ and $d_*$ satisfying

\[
\begin{bmatrix}
    c_* \\
    d_*
\end{bmatrix} =
\begin{bmatrix}
    M^{-1} H_k^* H_k & t (R_k^* A^* A W_k)^{-1} \\
    M^{-1} K_k^* K_k & t (R_k^* B^* B W_k)^{-1}
\end{bmatrix}
\begin{bmatrix}
    c \\
    d
\end{bmatrix}.
\]

Finally, the matrix above is invertible if

\[
t \det \begin{bmatrix}
    (R_k^* A^* A W_k)^{-1} & (R_k^* B^* B W_k)^{-1}
\end{bmatrix} \cdot \det \begin{bmatrix}
    R_k^* A^* A W_k M^{-1} H_k^* H_k & I \\
    R_k^* B^* B W_k M^{-1} K_k^* K_k & I
\end{bmatrix} \neq 0,
\]
where the first determinant is nonzero because its subblocks are invertible, and the second determinant equals

\[
\det(R_k^*A^*AW_kM^{-1}H_k^*H_k - R_k^*B^*BW_kM^{-1}K_k^*K_k) = \det(R_k^*R_k) \neq 0
\]

since \(R_k\) has full column rank. \(\square\)

Let \(r\) and \(s\) be two nonzero orthogonal vectors; then the locally optimal search direction in \(S = \text{span}\{r, s\}\) is the projection of the desired generalized singular vector \(x_1\) onto \(S\), and is given by

\[
r^*x_1 \frac{r^*r}{r^*r} + s^*x_1 \frac{s^*s}{s^*s}
\]

The remaining orthogonal direction in \(S\) is

\[
(x_1^*s)r - (x_1^*r)s,
\]

which is perpendicular to \(x_1\). It is usually impossible to compute the vectors from Proposition 5 and the linear combination in (13) without a priori knowledge of \(x_1\). Therefore, the idea is to pick \(r\) and \(s\) or \(a\) and \(b\) based on a different criterion, expand the search space with both vectors, and to rely on the extraction process to determine a good new search direction. If successful, then (14) suggests that there is at least one direction in the enlarged search space that is (nearly) perpendicular to \(x_1\). This direction may be removed to avoid excessive growth of the search space.

For example, we could use the approximate generalized singular pair and corresponding vectors from Section 2 and choose the vectors

\[
a = \bar{c}_1(I - W_kW_k^*)A^*\bar{x}_1 \quad \text{and} \quad b = \bar{c}_1(I - W_kW_k^*)B^*\bar{x}_1
\]

for expansion, and set

\[
r = a - b \quad \text{and} \quad s = (r^*b)a - (r^*a)b,
\]

since the residual norm \(\|r\|\) is required anyway. Moreover, this choice ensures at least the same improvement per iteration as the residual expansion from generalized Davidson. After the expansion and extraction, a low-quality search direction may be removed. Below we describe the process in more detail.

In Section 2 we have seen that \(A^*\bar{x}_1 = \bar{c}_1A^*\bar{u}_1\) and \(B^*\bar{x}_1 = \bar{s}_1B^*\bar{v}_1\); hence, suppose that \(W_{k+2}\) is obtained by extending \(W_k\) with the \(A^*\bar{u}_1\) and \(B^*\bar{v}_1\) after orthonormalization. Then we can compute the reduced QR-decompositions

\[
(15) \quad AW_{k+2} = U_{k+2}H_{k+2} \quad \text{and} \quad BW_{k+2} = V_{k+2}K_{k+2},
\]

and the triangular-form GSVD

\[
H_{k+2} \begin{bmatrix} \bar{w}_{k+1} \\ \bar{w}_{k+2} \end{bmatrix} = \begin{bmatrix} \bar{U}_{k+1} \\ \bar{U}_{k+2} \end{bmatrix} \begin{bmatrix} \bar{C}_{k+1} \\ \bar{C}_{k+2} \end{bmatrix} \begin{bmatrix} \bar{R}_{k+1} \\ \bar{R}_{k+1,k+2} \end{bmatrix},
\]

\[
K_{k+2} \begin{bmatrix} \bar{w}_{k+1} \\ \bar{w}_{k+2} \end{bmatrix} = \begin{bmatrix} \bar{V}_{k+1} \\ \bar{V}_{k+2} \end{bmatrix} \begin{bmatrix} \bar{S}_{k+1} \\ \bar{S}_{k+2} \end{bmatrix} \begin{bmatrix} \bar{T}_{k+1} \\ \bar{T}_{k+1,k+2} \end{bmatrix},
\]

where we may assume without loss of generality that \((\bar{c}_{k+2}, \bar{s}_{k+2})\) is the generalized singular pair furthest from the desired pair. By combining the partitioned decompositions above with (15), we see that the objective becomes the removal of \(\text{span}\{W_{k+2}\bar{w}_{k+2}\}\) from the search space. One way to
truncation unwanted direction from the search space, is to perform a restart conform Section 2
and compute

\[(16) \quad U_{k+2} \tilde{U}_{k+1}, \quad V_{k+2} \tilde{V}_{k+1}, \quad W_{k+2} \tilde{W}_{k+1}, \quad \tilde{c}_{k+2}, \text{ and } \tilde{s}_{k+2}, \]

explicitly. However, with \(O(nk^2)\) floating-point operations per iteration, the computational cost of
this approach is too high. The key to a faster method is to realize that we only need to be able to
truncate this unwanted direction from the search space, is to perform a restart conform Section 2
and compute

\[U_{k+2} \tilde{u}_{k+2}, \quad V_{k+2} \tilde{v}_{k+2}, \quad W_{k+2} \tilde{w}_{k+2}, \quad \tilde{c}_{k+2}, \text{ and } \tilde{s}_{k+2}, \]

but do not require the matrices in (16). To this end, let \(P, Q, \) and \(Z\) be Householder reflections of the
form

\[P = I - 2 \frac{pp^*}{p^*p}, \quad Q = I - 2 \frac{qq^*}{q^*q}, \quad \text{and } Z = I - 2 \frac{zz^*}{z^*z}, \]

with \(p, q, \) and \(z\) such that

\[P e_{k+2} = \tilde{u}_{k+2}, \quad Q e_{k+2} = \tilde{v}_{k+2}, \quad \text{and } Z e_{k+2} = \tilde{w}_{k+2}. \]

Applying the Householder matrices yields

\[(17) \quad A(W_{k+2}Z) = (U_{k+2}P)(P^*H_{k+2}Z) \quad \text{and} \quad B(W_{k+2}Z) = (V_{k+2}Q)(Q^*K_{k+2}Z), \]

which can be computed in \(O(nk)\) through rank-1 updates. It is straightforward to verify that the
bottom rows of \(P^*H_{k+2}Z\) and \(Q^*K_{k+2}Z\) are multiples of \(e_{k+2}^*\), e.g.,

\[e_{k+2}^*P^*H_{k+2}Z = \tilde{u}_{k+2}^* (\tilde{U}CR\tilde{W}^*)Z = \tilde{c}_{k+2}R_{k+2}^2 \tilde{w}_{k+2}^*Z = \tilde{c}_{k+2}2R_{k+2}^2 e_{k+2}^*. \]

As a result, (17) can be partitioned as

\[A \begin{bmatrix} W_{k+1} & W_{k+2} \tilde{w}_{k+2} \end{bmatrix} = \begin{bmatrix} U_{k+1} & U_{k+2} \tilde{u}_{k+2} \end{bmatrix} \begin{bmatrix} H_{k+1} & \times \\ \times \end{bmatrix} \begin{bmatrix} \tilde{c}_{k+2}2R_{k+2}^2 \end{bmatrix}, \]

\[B \begin{bmatrix} W_{k+1} & W_{k+2} \tilde{w}_{k+2} \end{bmatrix} = \begin{bmatrix} V_{k+1} & V_{k+2} \tilde{v}_{k+2} \end{bmatrix} \begin{bmatrix} K_{k+1} & \times \\ \times \end{bmatrix} \begin{bmatrix} \tilde{c}_{k+2}2R_{k+2}^2 \end{bmatrix}, \]

defining \(U_{k+1}, V_{k+1}, W_{k+1}, H_{k+1}, \) and \(K_{k+1}.\) This partitioning can be truncated to obtain

\[(18) \quad AW_{k+1} = U_{k+1}H_{k+1} \quad \text{and} \quad BW_{k+1} = V_{k+1}K_{k+1}, \]

where \(U_{k+1}, V_{k+1}, \) and \(W_{k+1}\) have orthonormal columns, but \(H_{k+1}\) and \(K_{k+1}\) are not necessarily
upper-triangular. The algorithm is summarized below in Algorithm 3.

**Algorithm 3** (Multidirectional GSVD (MDGSVD)).

**Input:** Matrix pair \((A, B),\) starting vectors \(w_1\) and \(w_2,\) minimum and maximum dimensions \(j < \ell.\)

**Output:** \(AW_j = U_jC_jR_j\) and \(BW_j = V_jS_jR_j\) approximating a partial GSVD.

1. Set \(W_0 = [\].\)
2. for number of restarts and not converged (cf., e.g., (8)) do
3. for \(k = 0, 1, \ldots, \ell - 2\) do
4. Let \(w_{k+1} = (I - W_kW_k^*)w_{k+1},\) and \(w_{k+1} = w_{k+1}/\|w_{k+1}\|\).
5. Let \(w_{k+2} = (I - W_kW_{k+1}^*)w_{k+2}\) and \(w_{k+2} = w_{k+2}/\|w_{k+2}\|\).
6. Update the QR-decompositions

\[AW_{k+2} = U_{k+2}H_{k+2}\text{ and } BW_{k+2} = V_{k+2}K_{k+2}.\]
Compute the GSVD $H_{k+2} = \tilde{U}C\tilde{R}W^*$ and $K_{k+2} = \overline{VS}\overline{R}W^*$.  

Let $P$, $Q$, and $Z$ be Householder reflections such that 
\[ Pe_{k+2} = \tilde{u}_{k+2}, \quad Qe_{k+2} = \tilde{v}_{k+2}, \quad \text{and} \quad Ze_{k+2} = \overline{z}_{k+2}. \]

Let $U_{k+2} = U_{k+2}P$, $V_{k+2} = V_{k+2}Q$, $W_{k+2} = W_{k+2}Z$, 
\[ H_{k+2} = P^*H_{k+2}Z, \quad \text{and} \quad K_{k+2} = Q^*K_{k+2}Z. \]

\[ \omega_{k+2} = A^*\tilde{u}_1 \quad \text{and} \quad \omega_{k+3} = B^*\overline{v}_1. \]

\[ \text{if } j \leq k \text{ and converged (cf., e.g., (8)) then break} \]

\[ \text{end} \]

Partition $\tilde{U}$, $\tilde{V}$, $\tilde{W}$, $\overline{C}$, $\overline{S}$, and $\overline{R}$ according to (6).

Let $U_j = U_j\tilde{U}_1$, $V_j = V_j\tilde{V}_1$, and $W_j = W_j\tilde{W}_1$.

Let $H_j = \tilde{C}_1\overline{R}_{11}$ and $K_j = \tilde{S}_1\overline{R}_{11}$.

\[ \text{end} \]

Algorithm 3 is a simplified description for the sake of clarity. For instance, the expansion vectors may be linearly dependent in practice, and it may be desirable to expand a search space of dimension $\ell - 1$ with only the residual instead of two vectors. Another missing feature that might be required in practice is deflation, which is the topic of the next section.

## 5 Deflation and the truncated GSVD

Deflation is used in eigenvalue computations to prevent iterative methods from recomputing known eigenpairs. Since Algorithm 1 and Algorithm 3 compute generalized singular values and vectors one at a time, deflation may be necessary for applications where more than one generalized singular pair is required. The truncated GSVD is an example of such an application. There are at least two ways in which generalized singular values and vectors can be deflated, namely by transformation and by restriction. These two approaches have been inspired by their counterparts for the symmetric eigenvalue problem (cf., e.g., Parlett [18, Ch. 5]). We only describe the two approaches for $m, p \geq n$ to avoid clutter, but note that they can be adapted to the general case.

The restriction approach is related to the truncation described in the previous section and may be used to deflate a single generalized singular pair at a time. Suppose we wish to deflate the simple pair $(c_1, s_1)$ and let the GSVD of $(A, B)$ be partitioned as 

\[
A = \begin{bmatrix} u_1 & U_2 \end{bmatrix} \begin{bmatrix} c_1 & r_{11}^* \ r_{12}^* & R_{22} \end{bmatrix} \begin{bmatrix} u_1^* \\ W_2^* \end{bmatrix} \\
B = \begin{bmatrix} v_1 & V_2 \end{bmatrix} \begin{bmatrix} s_1 & r_{11}^* \ r_{12}^* & R_{22} \end{bmatrix} \begin{bmatrix} v_1^* \\ W_2^* \end{bmatrix},
\]

where $C_2$ and $S_2$ may be rectangular. Then, with Householder reflections $P$, $Q$, and $Z$, satisfying 

\[
Pc_1 = e_1, \quad Qs_1 = e_1, \quad \text{and} \quad Zw_1 = e_1,
\]

it holds that 

\[
Pc_1R_{11} = A \times \hat{A} \quad \text{and} \quad Qs_1R_{11} = B \times \hat{B},
\]

defining $\hat{A}$ and $\hat{B}$. At this point, the generalized singular pairs of $(\hat{A}, \hat{B})$ are the generalized singular pairs of $(A, B)$ other than $(c_1, s_1)$. Additional generalized singular pairs can be deflated inductively.
An alternative that allows for the deflation of multiple generalized singular pairs simultaneously is the restriction approach. To derive this approach, let the GSVD of $(A, B)$ be partitioned as

\[
A = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} C_1 & \alpha \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} \\ \end{bmatrix} \begin{bmatrix} W_1^* \\ W_2^* \end{bmatrix}, \\
B = \begin{bmatrix} V_1 & V_2 \end{bmatrix} \begin{bmatrix} S_1 & \beta \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} \\ \end{bmatrix} \begin{bmatrix} W_1^* \\ W_2^* \end{bmatrix},
\]

where $C_1$ and $S_1$ are square and must be deflated, while $C_2$ and $S_2$ may be rectangular and must be retained. Therefore, the desired generalized singular pairs are deflated by working with the operators

\[
\begin{align*}
\tilde{A} &= U_2 C_2 R_{22} W_2^* = U_2 U_2^* A W_2 W_2^* = (I - U_1 U_1^*) A (I - W_1 W_1^*), \\
\tilde{B} &= V_2 S_2 R_{22} W_2^* = V_2 V_2^* B W_2 W_2^* = (I - V_1 V_1^*) B (I - W_1 W_1^*),
\end{align*}
\]

restricted to $\mathcal{W}_2 = \text{span}\{W_2\}$. An important benefit of this approach is that the restriction may be performed implicitly during the iterations. For example, if (6) is such that

\[
U_k \tilde{U}_1 = U_1, \quad V_k \tilde{V}_1 = V_1, \quad W_k \tilde{W}_1 = W_1, \quad \tilde{C}_1 = C_1, \quad \tilde{S}_1 = S_1, \quad \text{and} \quad \tilde{R}_{11} = R_{11};
\]

then

\[
\tilde{A} W_k \tilde{W}_2 = U_k \tilde{U}_2 \tilde{C}_2 \tilde{R}_{22} \quad \text{and} \quad \tilde{B} W_k \tilde{W}_2 = V_k \tilde{V}_2 \tilde{S}_2 \tilde{R}_{22},
\]

where the right-hand sides are available without explicitly working with $\tilde{A}$ and $\tilde{B}$. In addition, if we define the approximations for the next generalized singular pair and corresponding vectors as

\[
\begin{align*}
\alpha &= e_1^T \tilde{C}_2 e_1, & \beta &= e_1^T \tilde{S}_2 e_1, & \rho &= e_1^T \tilde{R}_{22} e_1, \\
\tilde{u} &= U_k \tilde{U}_2 e_1, & \tilde{v} &= V_k \tilde{V}_2 e_1, & \tilde{w} &= W_k \tilde{W}_2 e_1,
\end{align*}
\]

cf. Section 2, and

\[
\tilde{x} = \rho^{-1} W_k \tilde{W} \begin{bmatrix} \tilde{R}_{11}^{-1} \tilde{R}_{12} e_1 \\ e_1 \end{bmatrix} = \rho^{-1} (W_k \tilde{W}_1 \tilde{R}_{11}^{-1} \tilde{R}_{12} e_1 + \tilde{w});
\]

then the residual

\[
\begin{align*}
r &= \rho^{-1} (\beta^2 \tilde{A} \tilde{A} - \alpha^2 \tilde{B} \tilde{B}) \tilde{w} = \alpha \beta (\beta \tilde{A} \tilde{A} \tilde{u} - \alpha \tilde{B} \tilde{B} \tilde{v}) \\
&= \alpha \beta (\beta \tilde{A} \tilde{A} \tilde{u} - \alpha \tilde{B} \tilde{B} \tilde{v}) = (\beta^2 \tilde{A} \tilde{A} - \alpha^2 \tilde{B} \tilde{B}) \tilde{x}
\end{align*}
\]

and expansion vector(s) can also be computed without $\tilde{A}$ and $\tilde{B}$.

It may be instructive to point out that the restriction approach for deflation corresponds to a splitting method for general form Tikhonov regularization described in [9] and references. This method separates the penalized part of the solution from the unpenalized part associated with the nullspace of the regularization operator, essentially deflating specific generalized singular values and vectors. Consider, for instance, the minimization problem

\[
\arg\min_x \|Ax - b\|^2 + \mu \|Bx\|^2
\]

for some $\mu > 0$. Assume for the sake of simplicity that $p \geq n$, adding zero rows to $B$ if necessary, and suppose that $W_1$ is a basis for the nullspace of $B$; then we obtain

\[
\begin{align*}
\|Ax - b\|^2 + \mu \|Bx\|^2 &= \|U_1 U_1^* A W_1 W_1^* x - (U_1 U_1^* b - U_1 U_1^* A W_2 W_2^* x)\|^2 \\
&\quad + \|U_2 U_2^* A W_2 W_2^* x - U_2 U_2^* b\|^2 + \mu \|V_2 V_2^* B W_2 W_2^* x\|^2 \\
\end{align*}
\]
by following the splitting approach and using that \( U_3U_2^*AW_1W_1^*x = 0 \). Furthermore, with \( y_1 = W_1^*x \) and \( y_2 = W_2^*x \), the first part of the right-hand side of (21) reduces to
\[
\|(U_1^*AW_1)y_1 - (U_1^*b - U_1^*AW_2^*y_2)\|^2 = \|R_{11}y_1 - U_1^*(b - AW_2^*y_2)\|^2,
\]
which vanishes for \( y_1 = R_{11}^{-1}U_1^*(b - AW_2^*y_2) \). The remaining part may be written as
\[
\|\hat{A}W_2^*y_2 - U_2U_2^*b\|^2 + \mu \|\hat{B}W_2^*y_2\|^2,
\]
where we recognize the deflated matrices from (20). A similar expression can be derived for deflation through restriction, but does not provide additional insight.

6 Error analysis

In this section we are concerned with the quality of the computed approximations, and develop Rayleigh–Ritz theory that is useful for the GSVD. In particular, we will generalize several known results for the \( n \times n \) standard Hermitian eigenvalue problem to the Hermitian positive definite generalized eigenvalue problem

\[(22) \quad Nx = \lambda Mx, \quad M > 0, \quad M = L^2,\]

with eigenvalues \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \). This generalized problem is applicable in our context with \( N = A^*A \) and \( M = X^*X^{-1} \) if we are interested in the largest generalized singular values, or with \( N = B^*B \) and \( M = X^*X^{-1} \) if we are interested in the smallest generalized singular values; and corresponds to the standard problem

\[(23) \quad L^{-1}NL^{-1}y = \lambda y, \quad y = Lx,\]

with the same eigenvalues. Hence, if the subspace \( \mathcal{W} \) is a search space for (22), then it is natural to consider \( \mathcal{Z} = LW \) as a search space for (23) and to associate every approximate generalized eigenvector \( w \in \mathcal{W} \) with an approximate eigenvector \( z = Lw \in \mathcal{Z} \). The corresponding Rayleigh quotients satisfy

\[(24) \quad \theta = \frac{w^*Nw}{w^*Mw} = \frac{z^*L^{-1}NL^{-1}z}{z^*z} \]

and define the approximate eigenvalue \( \theta \).

Key to extending results for the generalized problem (23) to results for the standard problem (22), is to introduce generalized sines, cosines, and tangents, with respect to the \( M \)-norm defined by \( \|x\|_M^2 = x^*Mx = \|Lx\|^2 \). Generalizations of these trigonometric functions have previously been considered by Berns–Müller and Spence [2], and the generalized tangent can also be found in [18, Thm. 15.9.3]; however, we believe the treatment and results presented here to be new. The regular sine for two nonzero vectors \( y \) and \( z \) can be defined as
\[
\sin(z, y) = \frac{\|(I - \frac{z^*z}{\|z\|^2})y\|}{\|y\|} = \frac{\|(I - \frac{y^*y}{\|y\|^2})z\|}{\|z\|},
\]
where it is easily verified that the above two expressions are equal indeed. Substituting \( Lx \) for \( y \) and \( Lw \) for \( z \) yields the \( M \)-sine defined by
\[
\sin_M(w, x) = \sin(Lw, Lx) = \frac{\|(I - \frac{ww^*M}{w^*Mw})x\|_M}{\|x\|_M} = \frac{\|(I - \frac{xx^*M}{x^*Mx})w\|_M}{\|w\|_M}.
\]
Again, it may be checked that the above two expressions are equal. The regular cosine is given by
\[
\cos(z, y) = \frac{\|zz^*y\|}{\|y\|} = \frac{\|yy^*z\|}{\|z\|} = \frac{|z^*y|}{\|z\|\|y\|},
\]
and with the same substitution we find the \( M \)-cosine
\[
\cos_M(w, x) = \cos(Lw, Lx) = \frac{\|ww^*Mw\|_M}{\|x\|_M} = \frac{\|xx^*Mx\|_M}{\|w\|_M\|x\|_M}.
\]
The \( M \)-tangent is now naturally defined as \( \tan_M(w, x) = \sin_M(w, x)/\cos_M(w, x) \). We can derive the \( M \)-sines, \( M \)-cosines, and \( M \)-tangents between subspaces and vectors with a similar approach. For instance, let \( W \) and \( LW \) denote bases for \( W \) and \( Z \), respectively; then
\[
\sin(z, y) = \frac{\|(I - yy^*)Z(Z^*)^{-1}Z^*y\|}{\|Z(Z^*)^{-1}Z^*y\|} \quad \text{and} \quad \cos(z, y) = \frac{\|Z(Z^*)^{-1}Z^*y\|}{\|y\|},
\]
so that
\[
\sin_M(Wv, x) = \sin(LW, Lx) = \frac{\|\left(I - xx^*M\right)W(W^*MW)^{-1}W^*Mx\|_M}{\|W(W^*MW)^{-1}W^*Mx\|_M},
\]
\[
\cos_M(Wv, x) = \cos(LW, Lx) = \frac{\|W(W^*MW)^{-1}W^*Mx\|_M}{\|x\|_M},
\]
and \( \tan_M(Wv, x) = \sin_M(Wv, x)/\cos_M(Wv, x) \). It is important to note that \( \sin_M, \cos_M, \) and \( \tan_M \) can all be computed without the matrix square root \( L \) of \( M \).

Since our \( M \)-sines, \( M \)-cosines, and \( M \)-tangents equal their regular counterparts, the extension of several known results for the standard problem (23) to results for the generalized problem (22) is immediate. Below is a selection of error bounds, where we assume that the largest generalized eigenpair \((\lambda_1, x_1)\) is simple and is approximated by the Ritz pair \((\theta_1, w_1)\) of (22) with respect to the search space \( W \).

**Proposition 6** (Generalization of, e.g., [18, Lemma 11.9.2]).
\[
\sin_M^2(w_1, x_1) \leq \frac{\lambda_1 - \theta_1}{\lambda_1 - \lambda_2}.
\]

**Proposition 7** (Generalization of [19, Thm. 2.1]).
\[
\lambda_1 - \theta_1 \leq (\lambda_1 - \lambda_n) \sin_M^2(W, x_1).
\]
The two propositions imply that \( w_1 \to x_1 \) when \( \theta_1 \to \lambda_1 \), with \( \theta_1 \) tending to \( \lambda_1 \) when \( \sin(W, x_1) \to 0 \). The next corollary is a straightforward consequence.

**Corollary 8** (Generalization of [19, Thm. 2.1]).
\[
\sin_M^2(w_1, x_1) \leq \frac{\lambda_1 - \lambda_n}{\lambda_1 - \lambda_2} \sin_M^2(W, x_1) = \left(1 + \frac{\lambda_2 - \lambda_n}{\lambda_1 - \lambda_2}\right) \sin_M^2(W, x_1).
\]
As a result of Corollary 8, we can expect \( \sin_M(w_1, x_1) \) to be close to \( \sin_M(W, x_1) \) if the eigenvalue \( \lambda_1 \) is well separated from the rest of the spectrum. A sharper bound can be obtained by generalizing the optimal bound from Sleijpen, Van den Eshof, and Smit [19].
Proposition 9 (Generalization of [19, Thm. 3.2]). Let \((\theta_j, w_j)\) denote the Ritz pairs of the generalized problem (22) with respect to \(W\), and define
\[
\delta_W = \min \sin_M(w_j, x_1)
\]
as the smallest of all \(M\)-sines between the Ritz vectors \(w_j\) and the generalized eigenvector \(x_1\). Furthermore, define for any \(\epsilon > 0\) the maximum
\[
\delta_k(\epsilon) = \max_{\dim(W) = k} \{ \delta_W \mid \sin_M(W, x_1) \leq \epsilon \}.
\]
If \((\theta_W, w_W)\) is the Ritz pair for which \(\delta_W\) is realized and \(0 \leq \epsilon < (\lambda_1 - \lambda_2)/\lambda_1 - \lambda_2\) and
\[
\delta^2_k(\epsilon) = \frac{1}{2}(1 + \epsilon^2) - \frac{1}{2}\sqrt{(1 - \epsilon^2)^2 - \kappa \epsilon^2} \quad \text{with} \quad \kappa = \frac{(\lambda_2 - \lambda_n)^2}{\lambda_1 - \lambda_2},
\]
for all \(k \in \{2, \ldots, n-1\}\).

The quantity \(\delta^2_k(\epsilon)\) is not particularly elegant, but is sharp and can be used to obtain the following upper bound, which is sharper than the bound in Corollary 8.

Corollary 10 (Generalization of [19, Cor. 3.3]). If the conditions in Proposition 9 are satisfied, then
\[
\sin_M^2(w_1, x_1) \leq \sin_M^2(W, x_1) + \frac{\kappa}{2} \tan_M^2(W, x_1).
\]

Now that we have extended a number of results for the standard problem (23) to the generalized problem (22), it may be worthwhile to bound the generalized sine \(\sin_M\) in terms of the standard sine.

Proposition 11. Let \(\kappa = \kappa(M)\) be the condition number of \(M\), then
\[
\frac{1}{\kappa} \sin^2(w, x) \leq \sin_M^2(w, x) \leq \frac{1}{4}(\kappa + 1)^2 \sin^2(w, x).
\]

Proof. Without loss of generality we assume \(\|w\| = \|x\| = 1\), so that \(\lambda_{\min}(M) \leq \|x\|_M^2 \leq \lambda_{\max}(M)\).

The first inequality follows from
\[
\sin_M^2(w, x) = \left\| (I - w^*w)(I - \frac{w^*w}{w^*Mw})x \right\|^2 
\leq \|x\|_M^2 \left\| (I - \frac{w^*w}{w^*Mw})x \right\|_M^2 \sin_M^2(w, x) \leq \frac{\lambda_{\max}(M)}{\lambda_{\min}(M)} \sin_M^2(w, x).
\]

For the second inequality, it follows from, e.g., [20] that
\[
\left\| I - \frac{ww^*M}{w^*Mw} \right\| = \left\| \frac{ww^*M}{w^*Mw} \right\| = \frac{\|Mw\|}{\|w^*Mw\|} = \cos^{-1}(w, Mw) = \mu^{-1},
\]
where \(\mu^{-1}\) is the inverse of the first anti-eigenvalue [4, Ch. 3.6]
\[
\mu = \min_{\|w\| = 1} \frac{w^*Mw}{\|Mw\|}.
\]
By applying Kantorovich’ inequality we find \[\mu^{-1} = \frac{1}{2} \left( \lambda_{\min}(M) + \lambda_{\max}(M) \right) = \frac{1}{2} \left( \kappa + 1 \right).\]

Finally, by combining the above and using
\[
\left( I - \frac{ww^* M}{w^* Mw} \right) = \left( I - \frac{ww^* M}{w^* Mw} \right) (I - ww^*) \]
we see that
\[
\sin^2_M(w, x) = \frac{\| (I - \frac{ww^* M}{w^* Mw}) x \|_2^2}{\| x \|_2^2} \leq \frac{\lambda_{\max}(M)}{\lambda_{\min}(M)} \left( I - \frac{ww^* M}{w^* Mw} \right) = \kappa \left( I - \frac{ww^* M}{w^* Mw} \right) \| x \|_2^2 \leq \frac{1}{4} (\kappa + 1)^2 \sin^2(w, x),
\]
which concludes the proof.

An interesting observation about \(\sin_M\) in the context of the GSVD is that \(\| f \|\) from Proposition 4 equals \(\sin_M(\tilde{\tau}_1, x_1)\) if \(M = A' A + B' B = X^{-1} X^{-1}\). Furthermore, it has been shown in the proof of Proposition 4 that the error in \(\tilde{c}_2 = \| A \tilde{x}_1 \|_2^2\) and \(\tilde{c}_1 = \| B \tilde{x}_1 \|_2^2\) is quadratic in \(\| f \|\). An alternative is to express the approximation error in terms of the residual. We have, for example, the following straightforward Bauer–Fike-type result.

**Proposition 12** (Bauer–Fike for the GSVD). Let \((\tilde{\tau}, \tilde{s})\) be an approximate generalized singular pair with corresponding generalized singular vector \(\tilde{X}\) and residual \(r = (\tilde{s}^2 A' A - \tilde{s}^2 B' B) \tilde{X}\); then there exists a generalized singular pair \((c_*, s_*)\) of \((A, B)\) such that
\[
|\tilde{s}^2 c_* - \tilde{s}^2 s_*| \leq \| X \|_2^2 \frac{\| r \|}{\| \tilde{X} \|}.
\]

**Proof.** The result follows from
\[
\frac{\| r \|}{\| \tilde{X} \|} \geq \sigma_{\min}(\tilde{s}^2 A' A - \tilde{s}^2 B' B)
= \sigma_{\min}(X^{-1} (\tilde{s}^2 \Sigma_A^T \Sigma_A - \tilde{s}^2 \Sigma_B^T \Sigma_B) X^{-1}) \geq \sigma_{\min}^2(X^{-1}) \min_j \tilde{s}_j^2 \end{align*}
\[
\| r \| \geq \sigma_1 \| X \|_2 \frac{\| r \|}{\| \tilde{X} \|} \geq \sigma_{\min}(\tilde{s}^2 A' A - \tilde{s}^2 B' B)
\]

An additional interesting observation is that if \(\tilde{c}\) and \(\tilde{s}\) are scaled such that \(\tilde{c}^2 + \tilde{s}^2 = c_*^2 + s_*^2 = 1\), and the generalized singular values are given by \(\tilde{\sigma} = \tilde{c}/\tilde{s}\) and \(\sigma_* = c_*/s_*\); then
\[
|s_*^2 c_* - \tilde{s}^2 s_*| = |s_*^2 - \tilde{s}^2| = |c_*^2 - \tilde{c}^2| = \left| \tilde{\sigma}^2 \frac{1 + \sigma_*^2 - \sigma_*^2}{1 + \sigma_*^2} \right|,
\]
with the conventions \(\infty/\infty = 1\) and \(\infty - \infty = 0\).

The bound in Proposition 12 may be rather pessimistic, and we expect asymptotic convergence of order \(\| r \|_2^2\) due to the relation with the symmetric eigenvalue problem. It turns out that the desired result is easily generalized using the \(M\)-sine and the \(M^{-1}\)-norm. Specifically, let \(\theta\) be defined as in (24) and define the residual norms
\[
\rho(z) = \| (L^{-1} NL^{-1} - \theta I) z \| \quad \text{and} \quad \rho_M(w) = \rho(Lw) = \| (N - \theta M) w \|_{M^{-1}};
\]
then we can immediately derive the following proposition.
Proposition 13 (Generalization of, e.g., [18, Thm. 11.7.1, Cor. 11.7.1]). Suppose \( \lambda_1 - \theta_1 < \theta_1 - \lambda_2 \); then
\[
\frac{\rho_M(w_1)}{\lambda_1 - \lambda_n} \leq \sin M(w_1, x_1) \leq \frac{\rho_M(w_1)}{\theta_1 - \lambda_2}
\]
and
\[
\frac{\rho_M^2(w_1)}{\lambda_1 - \lambda_n} \leq \lambda_1 - \theta_1 \leq \frac{\rho_M^2(w)}{\theta_1 - \lambda_2}.
\]

Having the \( M^{-1} \)-norm for the residual instead of the \( M \)-norm might be surprising; however, the former is a natural choice in this context; see, e.g., [18, Ch. 15]. Moreover, Proposition 13 combined with the norm equivalence
\[
\sigma^{-1}_{\max}(M) \|r\|^2 \leq \|r\|_M^2 \leq \sigma^{-1}_{\min}(M) \|r\|^2
\]
implies that the convergence of the generalized singular values must be of order \( \|r\|^2 \). This result is verified in an example in the next section.

7 Numerical experiments

In this section we compare our new algorithms to JDGSVD and Zha’s modified Lanczos algorithm by using tests similar to the examples found in [8] and Zha [23]. Additionally, we will apply Algorithm 1 and Algorithm 3 to general form Tikhonov regularization by approximating truncated GSVDs for several test problems. The first set of examples is detailed below.

Example 1. Let \( A = CD \) and \( B = SD \) be two \( n \times n \) matrices, where
\[
C = \text{diag}(c_j), \quad c_j = (n - j + 1)/(2n), \quad S = \sqrt{I - C^2}, \\
D = \text{diag}(d_j), \quad d_j = \lceil j/(n/4) \rceil + r_j,
\]
with \( r_j \) drawn from the standard uniform distribution on the open interval \((0, 1)\).

Example 2. Let \( C \) and \( S \) be the same as in Example 1. Furthermore, let \( A = UC\bar{D}W^* \) and \( B = VS\bar{D}W^* \), where \( U, V, \) and \( W \) are random orthonormal matrices, and \( \bar{D} = \text{diag}(\bar{d}_j) \) with
\[
\bar{d}_j = d_j - \min_{1 \leq j \leq n} d_j + 10^{-\kappa}.
\]

Three values for \( \kappa \) are considered, \( \text{(a) } \kappa = 6, \text{ (b) } \kappa = 9, \text{ and (c) } \kappa = 12 \).

Example 3. Let \( C \) and \( S \) be the same as in Example 1, and let \( \bar{D} \) be the same as in Example 2. Let \( f, g, \) and \( h \) be random vectors on the unit \((n - 1)\)-sphere, and set
\[
A = (I - 2ff^*)C\bar{D}(I - 2hh^*) \quad \text{and} \quad B = (I - 2gg^*)S\bar{D}(I - 2hh^*). 
\]

Note that \( I - 2ff^*, I - 2gg^*, \) and \( I - 2hh^* \) are Householder reflections.

Example 4. Let
\[
A = \text{sprand}(n, n, 1e-1, 1) \quad \text{and} \quad B = \text{sprand}(n, n, 1e-1, 1e-2),
\]
where \text{sprand} is the MATLAB function with the same name.
We generate the matrices from Examples 1–4 for \( n = 1000 \), allowing us to verify the results. For Algorithm 1 and Algorithm 3 we set the minimum dimension to 10, the maximum dimension to 30, and the maximum number of restarts to 100. For JDGSVD we use the same minimum and maximum dimensions in combination with a maximum of 10 and 1000 inner and outer iterations, respectively. Furthermore, we let JDGSVD use standard extraction to find the largest generalized singular value, and refined extraction to find the smallest generalized singular value. We have implemented Zha's modified Lanczos algorithm with LSQR, and let LSQR use the tolerance \( 10^{-12} \) and a maximum of \( \lceil 10 \sqrt{n} \rceil = 320 \) iterations. The maximum number of outer-iterations for the modified Lanczos algorithm is 100.

We run each test with 500 different starting vectors, and record the number of matrix-vector products required until an approximate generalized singular pair \((\tilde{c}, \tilde{s})\) satisfies

\[
|s^2 c_{\text{max}}^2 - \tilde{c}^2 \tilde{s}_{\text{max}}^2| < \tau \quad \text{or} \quad |s^2 c_{\text{min}}^2 - \tilde{c}^2 \tilde{s}_{\text{min}}^2| < \tau,
\]

where we use \( \tau = 10^{-3} \) for Zha’s modified Lanczos algorithm and \( \tau = 10^{-6} \) for the remaining algorithms. The median results are shown in Table 1. We notice that the convergence of Zha’s method is markedly slower here than in [23]. Additional testing has indicated that the difference is caused by the larger choice of \( n \), which in turn decreases the gap between the generalized singular pairs. JDGSVD does not require accurate solutions from the inner iterations and is significantly

| Alg | Ex | Cond | Zha | JDGSVD | GDGSVD | MDGSVD |
|-----|----|------|-----|--------|--------|--------|
|     |    |      | \( \sigma_{\text{max}} \) | \( \sigma_{\text{min}} \) | \( \sigma_{\text{max}} \) | \( \sigma_{\text{min}} \) | \( \sigma_{\text{max}} \) | \( \sigma_{\text{min}} \) |
| 1   | 1  | 4.97e+00 | 3390 | 1524 | 6188 | 580 | 3072 | 502 | 730 |
| 2a  | 2a | 3.99e+06 | 19082 | 2008 | 5396 | 992 | 2326 | 1054 | 622 |
| 2b  | 2b | 3.99e+09 | 19082 | 2008 | 5396 | 992 | 2326 | 1054 | 622 |
| 3a  | 3a | 3.99e+12 | 19082 | 2008 | 5396 | 992 | 2326 | 1054 | 622 |
| 3b  | 3b | 3.99e+12 | 19082 | 2008 | 5396 | 992 | 2326 | 1054 | 622 |
| 4   | 4  | 1.41e+00 | 1262 | 1262 | 1262 | 2334 | 244 | 2314 | 240 |

We run each test with 500 different starting vectors, and record the number of matrix-vector products required until an approximate generalized singular pair \((\tilde{c}, \tilde{s})\) satisfies

\[
|s^2 c_{\text{max}}^2 - \tilde{c}^2 \tilde{s}_{\text{max}}^2| < \tau \quad \text{or} \quad |s^2 c_{\text{min}}^2 - \tilde{c}^2 \tilde{s}_{\text{min}}^2| < \tau,
\]

where we use \( \tau = 10^{-3} \) for Zha’s modified Lanczos algorithm and \( \tau = 10^{-6} \) for the remaining algorithms. The median results are shown in Table 1. We notice that the convergence of Zha’s method is markedly slower here than in [23]. Additional testing has indicated that the difference is caused by the larger choice of \( n \), which in turn decreases the gap between the generalized singular pairs. JDGSVD does not require accurate solutions from the inner iterations and is significantly

![Figure 1](image-url)
faster, but fails to converge to a sufficiently accurate solution in the last example. Compared to JDGSVD, GDGSVD approximately reduces the number of matrix-vector multiplications by a factor of 2 for $\sigma_{\text{max}}$ and by a factor of 2 to 2.4 for $\sigma_{\text{min}}$, and has no problem finding a solution for the last example. MDGSVD performs only slightly worse than GDGSVD for the largest generalized singular pairs on average, but uses approximately 4 times fewer MVs than GDGSVD for the smallest generalized singular pairs in almost all tests.

Figure 2: The errors of the largest (left) and smallest (right) generalized singular pairs approximations compared to the square of the relative residual norm in the right-hand side of (8). The results are for Example 2a and MDGSVD.

Figure 1 shows the convergence of MDGSVD. The monotone behavior and asymptotic linear convergence of the method are clearly visible. We can also see that the asymptotic convergence is significantly better than the worst-case bound from Proposition 4. Figure 2 shows a comparison between the relative residual norm (8) and the convergence of the generalized singular pairs for Example 2a. The results for the other examples are similar, and are therefore omitted. Although the graphs belonging to the smallest generalized singular pairs suggest temporary misconvergence, the comparison still demonstrates that (8) is an asymptotically suitable indicator for the convergence of the generalized singular pairs. Moreover, the convergence of the generalized singular pairs appears to be quadratic in the residual norm.

Example 5. Given a large, sparse, and ill-conditioned matrix $A$, consider the problem of reconstructing exact data $x_\star$ from measured data $b = Ax_\star + e$, where $e$ is a noise vector. A regularized solution may be determined with general form Tikhonov regularization by computing

$$x_\mu = \arg \min_x \|Ax - b\|^2 + \mu \|Bx\|^2$$

for some operator $B$ with $\mathcal{N}(A) \cap \mathcal{N}(B) = \{0\}$, and some parameter $\mu > 0$. For the purpose of this example, we take several $n \times n$ matrices $A$ and length $n$ solution vectors $x_\star$ from Regularization Tools [5], and for $B$ we use the $(n-1) \times n$ finite difference operator

$$B = \begin{bmatrix} 1 & -1 \\ \vdots & \ddots & \ddots \\ -1 & 1 \end{bmatrix}.$$

The entries of the noise vectors $e$ are independently drawn from the standard normal distribution, after which the vector $e$ is scaled such that $\epsilon = \mathbb{E}[\|e\|] = 0.01\|b\|$. We select the parameters $\mu$ such that $\|Ax_\mu - b\| = \eta \epsilon$, where $\eta = 1 + 3.090232/\sqrt{2n}$ so that $\|e\| \leq \eta \epsilon$ with probability 0.999.

Consider Example 5, where we can write $x_\mu$ as

$$x_\mu = X(\Sigma_A^* \Sigma_A + \mu \Sigma_B^* \Sigma_B)^{-1} \Sigma_A^* b = \sum_{i=1}^n \frac{c_i}{c_i^2 + \mu s_i^2} x_{i}^u b.$$
Table 2: Truncated GSVD tests where only the nullspace of $B$ is deflated, and the iterations are terminated when the relative residual for the second largest generalized singular pair after $(1, 0)$ is sufficiently small. The columns **Rank** and **Eff. cond** contain the numerical rank and effective condition number of $A$; and $\sin(x_2, \tilde{x}_2)$ is a measure for the error in the approximation of the generalized singular vector corresponding to the second largest generalized singular pair.

| Alg  | Ex    | Rank     | Eff. cond  | GDGSVD $\sin(x_2, \tilde{x}_2)$ | Rel. Err. | MV | MDGSVD $\sin(x_2, \tilde{x}_2)$ | Rel. Err. | MV |
|------|-------|----------|------------|--------------------------------|-----------|----|--------------------------------|-----------|----|
| Baart| 1024  | 3.88e+12 |            | 1.25e−5                         | 2.25e−5   | 1632| 3.40e−6                         | 2.08e−5   | 72 |
| Deriv2-1 | 1024 | 1.27e+06 |            | 1.90e−5                         | 1.70e−5   | 4228| 7.92e−6                         | 2.75e−5   | 2074|
| Deriv2-2 | 1024 | 1.27e+06 |            | 1.51e−5                         | 3.90e−5   | 4228| 7.92e−6                         | 9.90e−6   | 2074|
| Deriv2-3 | 1024 | 1.27e+06 |            | 1.90e−5                         | 1.91e−3   | 4228| 7.92e−6                         | 1.22e−4   | 2074|
| Foxgood | 30   | 3.88e+12 |            | 2.90e−5                         | 1.15e−5   | 4148| 4.59e−5                         | 2.31e−5   | 2830|
| Gravity-1 | 45   | 5.80e+12 |            | 1.56e−5                         | 2.52e−4   | 3764| 1.06e−5                         | 9.97e−4   | 1750|
| Gravity-2 | 45   | 5.80e+12 |            | 1.56e−5                         | 5.88e−4   | 3764| 1.06e−5                         | 9.85e−4   | 1750|
| Gravity-3 | 45   | 5.80e+12 |            | 1.56e−5                         | 3.04e−4   | 3764| 1.06e−5                         | 3.77e−4   | 1750|
| Heat-1 | 587   | 6.18e+12 |            | 3.52e−5                         | 4.20e−2   | 4976| 9.48e−6                         | 7.16e−2   | 802 |
| Heat-5 | 1022  | 1.27e+03 |            | 1.18e−5                         | 5.73e−2   | 5036| 7.44e−6                         | 1.28e−1   | 616 |
| Phillips | 1024 | 2.90e+10 |            | 1.25e−5                         | 5.82e−3   | 4188| 7.87e−6                         | 1.58e−3   | 1762|
| Shaw   | 20    | 4.32e+12 |            | 2.98e−5                         | 2.24e−2   | 3644| 1.32e−5                         | 7.75e−3   | 2308|
| Wing   | 16    | 1.01e+12 |            | 1.61e−5                         | 1.39e−5   | 4992| 4.55e−5                         | 1.44e−4   | 3064|

Table 3: Truncated GSVD tests and results similar to Table 2, but in this case with the approximation of the five largest generalized singular pairs after the pair $(1, 0)$ corresponding to the nullspace of the regularization operator.

| Alg  | Ex | GDGSVD $\sin(x_2, \tilde{x}_2)$ | Rel. Err. | MV | MDGSVD $\sin(x_2, \tilde{x}_2)$ | Rel. Err. | MV |
|------|----|---------------------------------|-----------|----|---------------------------------|-----------|----|
| Baart | 1024 | 1.82e−6                         | 3.19e−6   | 1996| 2.61e−8                         | 1.51e−7   | 74 |
| Deriv2-1 | 1024 | 8.03e−6                         | 8.99e−6   | 6088| 6.54e−6                         | 1.08e−5   | 3604|
| Deriv2-2 | 1024 | 8.03e−6                         | 3.52e−6   | 6088| 6.54e−6                         | 4.03e−6   | 3604|
| Deriv2-3 | 1024 | 8.03e−6                         | 6.25e−5   | 6088| 6.54e−6                         | 4.25e−5   | 3604|
| Foxgood | 193e−6 | 6.91e−6                         | 3.36e−6   | 6808| 1.07e−5                         | 5.20e−6   | 5485|
| Gravity-1 | 193e−6 | 1.93e−6                         | 1.14e−5   | 5600| 4.85e−6                         | 4.10e−5   | 4012|
| Gravity-2 | 193e−6 | 1.93e−6                         | 3.11e−5   | 5600| 4.85e−6                         | 3.50e−5   | 4012|
| Gravity-3 | 193e−6 | 1.93e−6                         | 8.39e−6   | 5600| 4.85e−6                         | 1.86e−5   | 4012|
| Heat-1 | 270e−6 | 2.70e−6                         | 2.82e−2   | 7520| 5.14e−6                         | 4.74e−2   | 1948|
| Heat-5 | 792e−6 | 7.92e−6                         | 4.63e−2   | 6676| 2.92e−6                         | 2.48e−2   | 1804|
| Phillips | 474e−6 | 4.74e−6                         | 3.49e−4   | 5912| 2.30e−6                         | 1.63e−4   | 3574|
| Shaw   | 191e−6 | 1.91e−6                         | 6.51e−5   | 5772| 2.67e−6                         | 1.80e−4   | 5620|
| Wing   | 833e−6 | 8.33e−6                         | 4.16e−6   | 5292| 1.44e−5                         | 7.26e−6   | 4618|

21
For large-scale problems with rapidly decaying $c_i$ and multiple right-hand sides $b$, it may be attractive to approximate the truncated GSVD and compute the above summation only for a few of the largest generalized singular pairs and their corresponding generalized singular vectors. In particular, we use our GDGSVD and MDGSVD methods to approximate the truncated GSVD consisting of the 15 largest generalized singular pairs and vectors. We use minimum and maximum dimensions 15 and 45, respectively, and a maximum of 100 restarts. We deflate or terminate when the right-hand side of (8) is less than $10^{-6}$, and seed the search space with the nullspace of $B$ spanned by the vector $(1, \ldots, 1)^T$. We consider two different cases. In the first case, we deflate the seeded vector and terminate as soon as the relative residual for the second largest generalized singular pair is sufficiently small. In the second case we deflate the seeded vector plus four additional vectors, and terminate when the relative residual corresponding to the sixth largest generalized singular pair is less than $10^{-6}$. We use the approximated truncated GSVDs to compute $x_\mu$, and compare it with the solution obtained with the exact truncated GSVD.

The experiments are repeated with 1000 different initial vectors and noise vectors, and the median results are reported in Table 2 and Table 3. Test problems Deriv2-{1,2,3} all use the same matrix $A$, but have different right-hand sides and solutions; the same is true for Gravity-{1,2,3}. Test problems Heat-{1,5} have the same solutions, but different $A$ and $b$. The tables show a reduction in the required number of matrix-vector products for multidirectional subspace expansion, with reduction factors approximately between 1.25 to 2.15 or better in the majority of cases. However, the reduced number of matrix-vector products may come at the cost of an increased relative error in the reconstructed solution and an increased angle between the exact and approximated generalized singular vector $x_2$, although not consistently.

8 Conclusion

We have discussed two iterative methods for the computation of a few extremal generalized singular values and vectors. The first method can be seen as a generalized Davidson-type method, and the second as a further generalization. Specifically, the second method uses multidirectional subspace expansion combined with a truncation phase to find improved search directions, while ensuring moderate subspace growth. Both methods allow for a natural and straightforward thick restart. We have also derived two different methods for the deflation of generalized singular values and vectors.

We have characterized the locally optimal search directions and expansion vectors in both the generalized Davidson method and the multidirectional method. Note that these search directions generally cannot be computed during the iterations. The inability to compute these optimal search directions motivates multidirectional subspace expansion and its reliance on the extraction process, as well as the removal of low-quality search directions. We have argued that our methods can still achieve (asymptotic) linear convergence and have provided asymptotic bounds on the rate of convergence. Additionally, we have shown that the convergence of both methods is monotonic, and have concluded the theoretical analysis by developing Rayleigh–Ritz theory and generalizing known results for the Hermitian eigenvalue problem to the Hermitian positive definite generalized eigenvalue problem that corresponds to the GSVD.

The theoretical convergence behavior is supported by our numerical experiments. Moreover, the numerical experiments demonstrate that our generalized Davidson-type method is competitive with existing methods, and suitable for approximating the truncated GSVD of matrix pairs with rapidly decaying generalized singular values. Significant additional performance improvements may be obtained by our new multidirectional method.
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