
UTV Expansion Pack

Special-Purpose

Rank Revealing Algorithms

Version 1.0 for MATLAB 6.5

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April 2004

CONTENTS

| | | |
|----------|--|-----------|
| 1 | Introduction | 7 |
| 2 | The Symmetric VSV Decomposition | 9 |
| 2.1 | Definitions | 9 |
| 2.2 | Algorithms | 10 |
| 2.3 | Hypernormal Rotations and Their Break-Down | 11 |
| 2.4 | Block QR Refinement | 12 |
| 2.5 | Rank-One Modifications | 12 |
| 3 | The Gap-Revealing QLP Factorization | 15 |
| 4 | The ULLIV Decomposition | 17 |
| 5 | A Lanczos Algorithm with Reorthogonalization and Restarts | 21 |
| 6 | Numerical Examples | 25 |
| 7 | Overview of Routines | 31 |
| | agl5 | 33 |
| | app_hyp | 34 |
| | app_qrot | 35 |
| | gen_hyp | 36 |
| | gen_qrot | 37 |
| | getrtzp | 38 |
| | hqlp | 39 |
| | hvsvid_L | 40 |
| | hvsvid_R | 41 |
| | hvsvid_cdef | 42 |
| | hvsvid_rdef | 43 |
| | hvsvsd | 44 |
| | lqlp | 45 |
| | lsdrr | 47 |
| | lvsvd | 48 |
| | lvsvd_cdef | 49 |
| | lvsvsd | 50 |
| | TOTinviter | 52 |
| | TOTlanczos | 53 |
| | TOTpowiter | 54 |
| | tprod | 55 |

| | |
|-----------------------|----|
| tprodinit | 56 |
| tvsv | 57 |
| ulliv | 58 |
| ulliv_up_a | 60 |
| ulliv_up_B | 62 |
| vsv_qrit | 64 |
| vsvid_L_mod | 65 |
| vsvid_R_mod | 66 |
| vsvid_ip | 67 |
| vsvsd_up | 68 |

ABSTRACT

This collection of Matlab software supplements and complements the package UTV TOOLS from 1999, and includes implementations of special-purpose rank-revealing algorithms developed since the publication of the original package. We provide algorithms for computing and modifying symmetric rank-revealing VSV decompositions, we expand the algorithms for the ULLV decomposition of a matrix pair to handle interference-type problems with a rank-deficient covariance matrix, and we provide a robust and reliable Lanczos algorithm which – despite its simplicity – is able to capture all the dominant singular values of a sparse or structured matrix. These new algorithms have applications in signal processing, optimization and LSI information retrieval. The corresponding manuscript is:

- R. D. Fierro and P. C. Hansen, *UTV Expansion Pack: Special-Purpose Rank-Revealing Algorithms*, submitted to Numerical Algorithms.

Acknowledgements

This work was supported by travel grants from Julie Damms Studiefond and Jubilæumsfonden ved DTU. The routine `lqlp` was written by David Huckaby, and we acknowledge the permission to include it here. We also thank Nicholas J. Higham for permission to include routines `cholp` and `ldlt_symm` from his Matrix Computation Toolbox.

1. INTRODUCTION

The Matlab package UTV Tools [5] from 1999 provides a collection of algorithms for computing and modifying (i.e., up- and downdating) rank-revealing decompositions of general matrices. These decompositions have many applications in signal processing, where they are used as fast and reliable alternatives [9], [20] to the versatile but computationally expensive and hard-to-update singular value decomposition (SVD).

Since the publication of UTV Tools more work has been done in the area of rank-revealing decompositions and algorithms. This work is motivated by the interest in using specialized rank-revealing algorithms, designed to take advantage of the underlying structure of the problem in consideration. The present package provides Matlab implementations of some of these newly developed algorithms, with emphasis on algorithms that expand the application areas of the original package (hence the name of the new package). Similar to the first package, the routines in this package can be considered as templates for more specialized implementations, perhaps in other computer languages, that can exploit the computer hardware.

Symmetric rank-revealing VSV decompositions for semidefinite and indefinite matrices were developed in [13] and [16] to provide algorithms and decompositions that take into account the symmetry of the matrix. Compared to the general UTV decompositions, the VSV decompositions lead to savings in computer time as well as advantages in the approximation properties of reduced-rank matrix approximations derived from the symmetric decompositions. The rank and subspace information provided by the VSV decompositions have applications, e.g., in deflation methods for solving block-structured symmetric indefinite systems [7] arising in optimization algorithms and PDE solvers.

The rank-revealing ULLV decomposition was originally developed for revealing the rank of a matrix quotient, defined as the product of one matrix and the pseudoinverse of another matrix, and with applications in noise reduction problems with broadband noise where the noise covariance matrix has full rank. When the noise covariance matrix is rank deficient (which is the case for interference or narrow-band noise) then the correct matrix quotient involves a weighted pseudoinverse [10], and the corresponding ULLV decomposition must reflect this. The most convenient way to deal with the full-rank and the rank deficient cases is to provide two different ULLV algorithms for the two variations of the decomposition.

While rank-revealing decompositions are convenient tools for dense matrices, they may be less suited for large sparse or structured matrices. For this reason we also provide a Lanczos algorithm for computing the dominant singular triplets of a matrix. Our algorithm demonstrates that if such an algorithm is based on complete reorthogonalization and explicit restarts, then the code need not be very complicated. The core of our implementation requires less than 100 lines of Matlab code, has a simple structure, and is thus suited for implementation on dedicated hardware platforms (in contrast to many other sophisticated – and much more general – implementations in mathematical software libraries).

In addition to the above algorithms, and for completeness, we provide implementations of a few simple and “heuristic” algorithms which will often reveal the numerical rank, but

without the safety (and slight overhead) of a genuine rank-revealing algorithm.

Finally we provide a few scripts that demonstrate the use of our functions in connection with rank-deficient KKT systems in optimization, noise and interference reduction in signal processing, and signal extraction in NMR signals.

In the following sections we summarize the algorithms, giving new theory where it is needed. We conclude with a few numerical examples and an overview of the new package. Throughout the paper, the norm $\|\cdot\|$ denotes the 2-norm, while I and E denote the identity matrix and the exchange matrix (consisting of the columns of the identity matrix in reverse order). Moreover, L and R always denote lower and upper triangular matrices, V is always an orthogonal matrix, and Ω is always a signature matrix. We also make use of Matlab's colon notation to indicate submatrices.

2. THE SYMMETRIC VSV DECOMPOSITION

The rank-revealing VSV decomposition of a symmetric matrix was first discussed by Luk and Qiao [16] (for Toeplitz matrices). A careful study of various algorithms based on initial triangular factorization can be found in [13], while a study of the accuracy of approximations based on the VSV decomposition is given in [4]

2.1. Definitions

Assume that the symmetric matrix $A \in \mathbb{R}^{n \times n}$ has numerical rank k , i.e., there is a well-defined gap between the k th singular value σ_k and the next. Then the rank-revealing VSV decomposition of A takes the form

$$A = V S V^T, \quad S = \begin{pmatrix} S_{11} & S_{12} \\ S_{12}^T & S_{22} \end{pmatrix}, \quad V = (V_1, V_2), \quad (2.1)$$

where the symmetric matrix S is partitioned such that it reveals the numerical rank of A , i.e., the singular values of the $k \times k$ leading submatrix S_{11} approximate the first k singular values of A , while the norms $\|S_{12}\|$ and $\|S_{22}\|$ of the off-diagonal and trailing blocks are both of the order σ_{k+1} , cf. [13], [16].

The matrix V is orthogonal, and it is partitioned such that the column spaces of the two blocks V_1 and V_2 are approximations to the subspaces spanned by the first k and the last $n - k$ right singular vectors of A , respectively. In the signal processing literature, these two subspaces are referred to as the signal and noise subspaces. See [4] concerning the accuracy of these approximations.

For practical purposes, we choose to compute and represent the matrix S in the factored form

$$S = T^T \Omega T, \quad (2.2)$$

in which T is an upper or lower triangular matrix, and Ω is a signature matrix, i.e., a diagonal matrix with ± 1 on the diagonal, such that the inertia of A is preserved in the inertia of Ω . If A is positive definite then Ω is the identity matrix.

For semidefinite matrices, it was found in [13] that the optimal form of T is lower triangular, because this choice leads to more accurate approximations of the signal and noise subspaces. Our package therefore includes software for computing the VSV decomposition $A = V L^T L V^T$ of a symmetric semidefinite matrix. We provide two functions `hvsbsd` and `lvsvsd`, optimized for the high-rank case ($k \approx n$) and low-rank case ($k \ll n$), respectively.

For indefinite matrices, the singular vector estimation (which is part of the VSV algorithm) is simpler when T is upper triangular, while a lower triangular T provides a decomposition that is consistent with the semidefinite case. We provide high-rank VSV algorithms for both forms: the functions `hvsvid_L` and `hvsvid_R` compute the lower triangular form $A = V L^T \Omega L V^T$ and the upper triangular form $A = V R^T \Omega L R^T$, respectively. In the

LOW-RANK VSV ALGORITHM `lvsvd`:

1. Compute $A = V L^T \Omega L V^T$ and let $k \leftarrow 1$.
2. Condition estimation: let $\tilde{\sigma}_k$ estimate $\|L(k:n, k:n)^T \Omega(k:n, k:n) L(k:n, k:n)\|$ and let w_k estimate the corresponding right singular vector.
3. If $\tilde{\sigma}_k < \tau$ then $k \leftarrow k - 1$, **exit**.
4. Revelement: determine orthogonal P_k such that $P_k^T w_k = (1, 0, \dots, 0)^T$;
5. update $L(k:n, k:n) \leftarrow L(k:n, k:n) P_k$ and $V(:, k:n) \leftarrow V(:, k:n) P_k$;
6. update $L(k:n, k:n) \leftarrow Q_k^T L(k:n, k:n)$, $\Omega(k:n, k:n) \leftarrow Q_k^T \Omega(k:n, k:n) Q_k$, where the hypernormal Q_k ensures that the updated L is triangular.
7. Deflation: let $k \leftarrow k + 1$.
8. Go to step 2.

HIGH-RANK VSV ALGORITHMS `hvsvid_T` WITH $T = L$ OR R :

1. Compute $A = V T^T \Omega T V^T$ and let $k \leftarrow 1$.
2. Condition estimation: let $\tilde{\sigma}_k$ estimate $\sigma_{\min}(T(1:k, 1:k)^T \Omega(1:k, 1:k) T(1:k, 1:k))$ and let w_k estimate the corresponding right singular vector.
3. If $\tilde{\sigma}_k > \tau$ then **exit**.
4. Revelement: determine orthogonal P_k such that $P_k^T w_k = (0, \dots, 0, 1)^T$;
5. update $T(1:k, 1:k) \leftarrow T(1:k, 1:k) P_k$ and $V(:, 1:k) \leftarrow V(:, 1:k) P_k$;
6. update $T(1:k, 1:k) \leftarrow Q_k^T T(1:k, 1:k)$ and $\Omega(1:k, 1:k) \leftarrow Q_k^T \Omega(1:k, 1:k) Q_k$, where the hypernormal Q_k ensures that the updated T is triangular.
7. Deflation: let $k \leftarrow k - 1$.
8. Go to step 2.

Figure 2.1: The VSV algorithms for symmetric indefinite matrices.

low-rank case the dilemma vanishes, and the function `lvsvd` computes the lower triangular form.

An alternative, but more expensive, approach to computing a high-rank indefinite VSV decomposition with a lower triangular T is to first compute the upper triangular form $A = V R^T \Omega R V^T$ and then compute the QR factorization $R^T = Q L^T$ which yields the lower triangular form $A = (VQ) L^T \Omega L (VQ)^T$. This approach is easy to implement using Matlab's `qr` function, but it is more expensive and therefore we do not provide an implementation.

2.2. Algorithms

The generic algorithm for computing the VSV decomposition of a symmetric semidefinite matrix is quite simple, because the singular values of T are the square roots of the singular values of A when $\Omega = I$. First we compute the symmetrically pivoted Cholesky factorization $\Pi A \Pi^T = \overline{C}^T \overline{C}$ (we use rook pivoting as implemented in [14]), followed by the computation of the rank-revealing ULV decomposition $E \overline{C} E = \widehat{U} L \widehat{V}^T$ (using high-rank and low-rank functions from UTV Tools). As a result, we obtain the desired decomposition $A = (\Pi \widehat{V}) L^T L (\Pi \widehat{V})^T$.

The generic algorithm for indefinite matrices starts with a symmetrically pivoted LDL^T factorization $\Pi A \Pi^T = \overline{L} \overline{D} \overline{L}^T$, using the rook pivoting implemented in [14]. Next, the middle block diagonal matrix \overline{D} is replaced by the signature matrix, $\overline{L} \overline{D} \overline{L}^T = \widehat{W} \widehat{L} \widehat{\Omega} \widehat{L}^T \widehat{W}^T$, where \widehat{W} is an orthogonal block diagonal matrix with 1×1 and 2×2 blocks on the diagonal; see §4.2 in [13].

Finally we reveal the rank of the product $\widehat{L}\widehat{\Omega}\widehat{L}^T$, by “peeling off” the small or large singular values one at a time. Our algorithms take basis in the following two reformulations and partitionings with $R = \widehat{L}^T$, $L = E\widehat{L}^T E$ and $\Omega = E\widehat{\Omega}E$:

$$\begin{aligned} R^T\widehat{\Omega}R &= \begin{pmatrix} R_{11}^T & 0 \\ R_{12}^T & R_{22}^T \end{pmatrix} \begin{pmatrix} \widehat{\Omega}_1 & 0 \\ 0 & \widehat{\Omega}_2 \end{pmatrix} \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix} \\ &= \begin{pmatrix} R_{11}^T\widehat{\Omega}_1R_{11} & R_{11}^T\widehat{\Omega}_1R_{12} \\ R_{12}^T\widehat{\Omega}_1R_{11} & R_{12}^T\widehat{\Omega}_1R_{12} + R_{22}^T\widehat{\Omega}_2R_{22} \end{pmatrix} \end{aligned} \quad (2.3)$$

$$\begin{aligned} L^T\Omega L &= \begin{pmatrix} L_{11}^T & L_{21}^T \\ 0 & L_{22}^T \end{pmatrix} \begin{pmatrix} \Omega_1 & 0 \\ 0 & \Omega_2 \end{pmatrix} \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \\ &= \begin{pmatrix} L_{11}^T\Omega_1L_{11} + L_{21}^T\Omega_2L_{21} & L_{21}^T\Omega_2L_{22} \\ L_{22}^T\Omega_2L_{21} & L_{22}^T\Omega_2L_{22} \end{pmatrix}. \end{aligned} \quad (2.4)$$

The indefinite VSV algorithms are summarized in Fig. 2.1. Following the ideas from [3] in the low-rank case, we can now determined orthogonal transformations such that they, when applied symmetrically to $L^T\Omega L$, ensure that the singular values of the (1,1)-block in (2.4) approximate the largest singular values of A . The construction of these transformations involves the computation of the largest singular value and corresponding right singular vector of the submatrix $L_{22}^T\Omega_2L_{22}$, and the user can choose between power iterations and the Lanczos method. At the same time, hypernormal rotations are used to maintain the triangular form of L .

In the high-rank case we follow the ideas from [16] and construct orthogonal transformations which ensure that the smallest singular values of A are revealed in the (2,2)-block in (2.3) and (2.4). This involves the computation of the smallest singular value and corresponding right singular vector of the (1,1)-block. In the upper triangular case (2.3) this is done by means of inverse iterations applied to the submatrix $R_{11}^T\widehat{\Omega}_1R_{12}$.

In the lower triangular case (2.4), however, it is impractical to apply inverse iterations to the submatrix $L_{11}^T\Omega_1L_{11} + L_{21}^T\Omega_2L_{21}$ because we do not have a useful factorization of this matrix. The inverse iterations are much easier to use when we can ignore the second term, but unfortunately this is not always the case: according to Thm. 4.3 in [13] $\|L_{21}^T\Omega_2L_{22}\|$ and $\|L_{22}^T\Omega_2L_{22}\|$ are guaranteed to be small, but this does not imply that $\|L_{21}^T\Omega_2L_{21}\|$ is small. Our solution is to apply a single step of block QR refinement to L , as described below; this ensures that the norm $\|L_{21}\|$ of the off-diagonal block in L is always small.

2.3. Hypernormal Rotations and Their Break-Down

Hypernormal transformations are introduced in [2], and their use in our VSV algorithms is discussed in [13]. The “building blocks” of hypernormal transformations are Givens and hyperbolic rotations, the latter performing the transformation (for $|\alpha| > |\beta|$):

$$\begin{pmatrix} c & -s \\ -s & c \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} (\alpha^2 - \beta^2)^{1/2} \\ 0 \end{pmatrix}$$

where $c^2 - s^2 = 1$. The hyperbolic transformation is not defined when $|\alpha| = |\beta|$, and it has large elements $|\alpha|$ and $|\beta|$ when $|\alpha|$ is close to $|\beta|$.

In our algorithms, the hyperbolic transformations are used to annihilate fill in the triangular matrix during the revelation steps (see Fig. 2.1). Consider the following situation,

where a right Givens rotation has introduced a nonzero element “*” in position $(i + 1, i)$:

$$\begin{array}{cccccc}
 & & \times & \times & \times & \times & \times & \times \\
 & & & \times & \times & \times & \times & \times \\
 i & \rightarrow & & & \times & \times & \times & \times \\
 i + 1 & \rightarrow & & & * & \times & \times & \times \\
 & & & & & & \times & \times \\
 & & & & & & & \times
 \end{array}$$

If the fill satisfies $|r_{i+1,i}| \approx |r_{ii}|$ then we introduce large elements in the updated R which cancel in the product $R^T \Omega R$; an undesirable situation in numerical computations. Our remedy is to detect this situation and resort to a “fix.” When $\||r_{i+1,i}| - |r_{ii}|\| < 10^{-5} \|R(i:i+1, i:i+1)\|$, we perform a cyclic permutation of columns i through $i + 2$, leading to the form

$$\begin{array}{cccccc}
 & & \times & \times & \times & \times & \times & \times \\
 & & & \times & \times & \times & \times & \times \\
 i & \rightarrow & & & \times & \times & \times & \times \\
 i + 1 & \rightarrow & & & \times & \times & * & \times \\
 & & & & & \times & & \times \\
 & & & & & & & \times
 \end{array}$$

after which we use hypernormal transformations to annihilate the two elements below the diagonal in columns i and $i + 1$. We then return to the condition estimation step and restart the revelation process. If we only permuted columns i and $i + 1$ then the difficulty would arise again in the restarted revelation step.

2.4. Block QR Refinement

In analogy with block QR refinement of UTV decompositions, we can apply a similar algorithm to the VSV decompositions in order to reduce the norm of the off-diagonal blocks. We discuss the algorithm for the upper triangular version only; the algorithm for the lower triangular version is practically the same.

Given R partitioned as in (2.3) we first apply a sequence of right orthogonal transformations to annihilate the submatrix R_{12} , thus filling out the elements in the (2,1)-block. These elements, in turn, are annihilated by means of left hypernormal transformations which create new elements in the (1,2)-block.

We now justify this approach when applied to $S = R^T \Omega R$. Let $R = L_B Q_B$ where L_B is lower block triangular and Q_B is orthogonal; then $S = (R^T \Omega L_B) Q_B$ and a block QR step consists of formally forming the product $S_B \equiv Q_B (R^T \Omega L_B) = L_B^T \Omega L_B$. Next, let $L_B = H_B R_B$ where R_B is upper triangular and H_B is hypernormal with $H_B^T \Omega H_B = \Omega_B$ (in which Ω_B is a new signature matrix). Inserting this we obtain $S_B = R_B^T \Omega_B R_B$, showing that the new factors R_B and Ω_B indeed correspond to performing a block QR step on S .

The block QR refinement is implemented in the function `vsv_qrit` which determines whether it is applied to a semidefinite or an indefinite matrix and, in the latter case, whether it is applied to the L or R version.

2.5. Rank-One Modifications

We also provide algorithms for rank-one modifications of the form

$$A' = A + \omega v v^T, \tag{2.5}$$

where $\omega = \pm 1$ and v a vector. Equation (2.5) can be recast as

$$A' = V \begin{pmatrix} T \\ v^T V \end{pmatrix}^T \begin{pmatrix} \Omega & 0 \\ 0 & \omega \end{pmatrix} \begin{pmatrix} T \\ v^T V \end{pmatrix} V^T.$$

When A is semidefinite and $\omega = 1$, the updating is equivalent to a rank-one update of the ULV decomposition where the numerical rank cannot decrease. The updating is implemented in function `vsvd_up` and uses functions from UTV Tools.

When $\omega = -1$ or when A is indefinite then the numerical rank of A' can stay the same, or it can increase or decrease by one. Then the updated factors are computed by applying left hypernormal rotations to annihilate the row $v^T V$. This modification algorithm is implemented in the two functions `vsvid_L_mod` and `vsvid_R_mod`.

For efficiency reasons one should avoid to apply the rank-revealing post processing to the full S matrix. We partition $v^T V = d^T = (d_1^T, d_2^T)$ according to (2.3) and apply right Givens rotations G such that

$$d_2^T G^T = e_2^T = (\|d_2\|, 0, \dots, 0)^T.$$

At the same time we apply left hypernormal rotations H to maintain the triangular form of the (2,2)-block. Introducing $R'_{12} = R_{12}G$, $R'_{22} = H^T R_{22}G$ and $\Omega'_2 = H^T \Omega_2 H$, we now have

$$\begin{aligned} V^T A' V &= \begin{pmatrix} I & 0 \\ 0 & G \end{pmatrix} \begin{pmatrix} R_{11} & R'_{12} \\ 0 & R'_{22} \\ d_1^T & e_2^T \end{pmatrix}^T \begin{pmatrix} \Omega_1 & 0 & 0 \\ 0 & \Omega'_2 & 0 \\ 0 & 0 & \omega \end{pmatrix} \begin{pmatrix} R_{11} & R'_{12} \\ 0 & R'_{22} \\ d_1^T & e_2^T \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & G \end{pmatrix}^T \\ &= \begin{pmatrix} R_{11}^T \Omega_1 R_{11} & R_{11}^T \Omega_1 R_{12} G + \omega d_1 e_2^T \\ G^T R_{12}^T \Omega_1 R_{11} + \omega e_2 d_1^T & G^T (R_{12}^T \Omega_1 R_{12} + R_{22}^T \Omega_2 R_{22}) G + \omega e_2 e_2^T \end{pmatrix}. \end{aligned}$$

Since $S = R^T \Omega R$ reveals the rank of A , we know that both norms $\|R_{11}^T \Omega_1 R_{12} G\| = \|R_{11}^T \Omega_1 R_{12}\|$ and $\|G^T (R_{12}^T \Omega_1 R_{12} + R_{22}^T \Omega_2 R_{22}) G\| = \|R_{12}^T \Omega_1 R_{12} + R_{22}^T \Omega_2 R_{22}\|$ are small. Hence, due to the structure of $d_1 e_2^T$ and $e_2 e_2^T$, it is not possible to have any elements of large magnitude in the last $n - k - 1$ rows or columns of the above matrix. Therefore, once d^T has been annihilated, it suffices to reveal the rank of the leading $(k+1) \times (k+1)$ submatrix of the updated S factor.

3. THE GAP-REVEALING QLP FACTORIZATION

Stewart [21] introduced the so-called QLP factorization

$$A = Q L P^T \tag{3.1}$$

in which Q and P are orthogonal, and L is lower triangular. The factorization is gap revealing in the sense that the absolute values of the diagonal elements of L often track the singular values of A ; but there is no guarantee that this is always the case. Hence, the factorization is not rank-revealing in the strict sense used in this package.

To compute the QLP decomposition, we compute a pivoted QR factorization $A \Pi_P = Q R$ followed by a second pivoted QR factorization $R^T \Pi_Q = P L^T$, and thus $A = (Q \Pi_Q) L (\Pi_P P)^T$. For high-rank matrices, this is easy to implement with Matlab's QR factorization, and it is implemented in function `hqlp`.

For low-rank matrices, Huckaby and Chan [15] implemented an algorithm using interleaved left and right Householder transformations. The algorithm essentially produces one row of L at a time, starting from the top, and stops as soon as a gap is revealed. At this stage, the heuristic is that if we compute the full QLP factorization then the norms of the (2,1)- and (2,2)-blocks of L will be small. Hence we can neglect these blocks and return the low-rank approximation

$$A_k = Q(:, 1:k) L(1:k, 1:k) P(:, 1:k)^T, \tag{3.2}$$

where the gap appears between singular values σ_k and σ_{k+1} . This algorithm is implemented in function `lqlp`, and we emphasize that it computes the rank- k matrix *approximation* in (3.2), not a full factorization.

4. THE ULLIV DECOMPOSITION

The ULLV decomposition of a matrix pair (A, B) with $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{p \times n}$ was originally defined for the case $m \geq n \geq \text{rank}(A)$ and $p \geq n = \text{rank}(B)$ in [17]. Algorithms for computing and modifying this decomposition are included in UTV Tools.

In certain applications, such as interference reduction [10], [12], the matrix B does not have full column rank. This led Luk and Qiao [18] to define an alternative decomposition, which we shall refer to as the ULLIV decomposition. Assume again that $m \geq n \geq \text{rank}(A)$ while B has full row rank, i.e., $\text{rank}(B) = p < n$. Then the ULLIV decomposition takes the form

$$A = U_A L_A \begin{pmatrix} L & 0 \\ 0 & I \end{pmatrix} V^T, \quad B = U_B (L, 0) V^T \quad (4.1)$$

in which I is an identity matrix of order $n - p$, $U_A \in \mathbb{R}^{m \times n}$ has orthonormal columns, and $U_B \in \mathbb{R}^{p \times p}$ and $V \in \mathbb{R}^{n \times n}$ are orthogonal. Moreover, $L_A \in \mathbb{R}^{n \times n}$ and $L \in \mathbb{R}^{p \times p}$ are both lower triangular.

As shown in [10], when $\text{rank}(B) < n$ it is the matrix quotient $A B_A^\dagger$ that is required, and whose numerical rank should be revealed. Here B_A^\dagger is the A -weighted pseudoinverse of B . Given the ULLIV decomposition (4.1) it is proved in [10] that

$$A B_A^\dagger = U_A L_A(1:p, 1:p) U_B^T,$$

showing that the leading $p \times p$ block of L_A must be rank revealing. To compute such a ULLIV decomposition, we start with the QR factorization $B = (L, 0) V^T$ followed by the QR factorization $A V \begin{pmatrix} L^{-1} & 0 \\ 0 & I \end{pmatrix} = U_A L_A$. Setting $U_B = I$ we thus have an initial decomposition, which is then made rank-revealing by applying the similar steps from the ULLV algorithm to L and U_B as well as to the first p columns of L_A , U_A and V . This algorithm is implemented in function `ulliv`.

An efficient algorithm for updating the ULLIV decomposition when a row a^T is appended to A is described in [18]. The algorithm takes its basis in the formulation

$$\begin{pmatrix} A \\ a^T \end{pmatrix} = \tilde{U}_A \begin{pmatrix} L_A \\ d^T \end{pmatrix} \begin{pmatrix} L & 0 \\ 0 & I \end{pmatrix} V^T, \quad B = U_B (L, 0) V^T$$

with

$$\tilde{U}_A = \begin{pmatrix} U_A & 0 \\ 0 & 1 \end{pmatrix}, \quad d^T = a^T V \begin{pmatrix} L^{-1} & 0 \\ 0 & I \end{pmatrix}.$$

In the first stage, the partial row $d(p+1:n)^T$ is annihilated by means of left Givens rotations which are absorbed in \tilde{U}_A ; these rotations maintain the small and rank-revealing elements in $L_A(1:p, 1:p)$. In the second stage, the remaining elements of the row d^T are annihilated by interleaved right and left Givens rotations – this stage is identical to the ULLV updating algorithm from UTV tools, and modifies U_B and L as well as the first p columns of \tilde{U}_A , L_A

5. A LANCZOS ALGORITHM WITH REORTHOGONALIZATION AND RESTARTS

We now describe our Lanczos-based routine `lsvdrr` for computing the largest p singular values σ_i and associated right singular vectors v_i of a matrix A . Our algorithm uses full reorthogonalization and explicit restarts, and it is based on the work in [6] with modifications that make it more reliable and possibly faster.

If we apply k steps of the Lanczos algorithm [8, §§9.1–2] to the matrix $A^T A$ (by first multiplying with A and then by A^T), cf. Fig. 5.1, then in exact arithmetic we produce an $n \times k$ matrix V_k with orthonormal columns, and a $k \times k$ symmetric semidefinite tridiagonal matrix T_k , such that $A V_k = V_k T_k$. Then it is well known that some of the large eigenvalues of T_k will approximate some of the large eigenvalues of $A^T A$. Since these eigenvalues are the squares of the singular values of A , we thus have a basic procedure for iteratively computing approximations to the large singular values of a matrix.

More precisely, let $T_k = S_k \Theta_k S_k^T$ denote the eigenvalue decomposition of T_k , and let $\theta_i^{(k)}$ denote these eigenvalues. Moreover, let $y_i^{(k)}$ denote the columns of the matrix $Y_k = V_k S_k$. Then $(\theta_i^{(k)}, y_i^{(k)})$ are called the Ritz pairs associated with the k th step of the Lanczos process, and some of the Ritz pairs will approximate some of the eigenpairs of $A^T A$.

Since this Lanczos algorithm is based on the implicit formation of the matrix $A^T A$, there is no guarantee that it can provide accurate estimates of the small singular values of A in finite-precision computations. This does not cause a problem here, however, because our algorithm is intended solely for the computation of the largest singular values.

A more severe difficulty with finite-precision computations in the Lanczos algorithm is that the Lanczos vectors (the columns of V_k) lose orthogonality as the Ritz values converge. This, in turn, leads to various difficulties with repeated and spurious eigenvalues of T_k that do not represent approximations to eigenvalues of $A^T A$. A number of sophisticated remedies have been proposed for overcoming these difficulties, many of them involving partial or selective reorthogonalizations, combined with methods for monitoring the accuracy of the Ritz values, cf. [8, §9.2]. With the inclusion of these techniques, the Lanczos algorithm can be used as a general-purpose method for computing, in principle, any portion of the eigenvalue spectrum of A .

Our goal here, on the other hand, is to provide a simple Lanczos algorithm solely for computing the largest p singular values of a matrix, suited as a basis for dedicated hardware implementations. For this reason, we use complete reorthogonalization among the Lanczos vectors (which takes place after step 5 in the `gettzip` algorithm in Fig. 5.1). As long as p is not large, the additional computational work involved in this approach is acceptable, the actual code is very simple, and the storage requirements for the Lanczos vectors and the converged Ritz vectors are known a priori.

Our stopping criterion for the Lanczos process is based on an estimate of the error in $(\theta_i^{(k)})^{1/2}$, when considered an approximation to σ_j ; different indices i and j are needed

BASIC LANCZOS ALGORITHM `getrtzp`:

1. Initialization: $\beta_0 \leftarrow 0$; $v_0 \leftarrow 0$; $v_1 \leftarrow$ initial vector.
2. For $k = 1, \dots, \ell$
3. $w \leftarrow A^T(A v_k) - \beta_{k-1} v_{k-1}$;
4. $T_{k,k} \leftarrow \alpha_k \leftarrow v_k^T w$;
5. $w \leftarrow \alpha_k v_k$;
6. $T_{k,k+1} = T_{k+1,k} \leftarrow \beta_k \leftarrow \|w\|$;
7. $v_{k+1} \leftarrow w / \beta_k$;
8. $T_k = S_k \Theta_k S_k^T$ (eigenvalue decomposition).
9. Use error estimates $e_i^{(k)}$ (5.1) to identify n_c converged Ritz pairs.

LANCZOS SVD ALG. w/ REORTHOGONALIZATION AND RESTARTS `lsvdrr`:

1. Initialization: $v_{\text{init}} \leftarrow A^T e$; $n_{\text{crp}} \leftarrow 0$; $\mathcal{RP} \leftarrow \emptyset$ (no Ritz pairs).
2. While $n_{\text{crp}} < k$
3. use `getrtzp` to compute n_c Ritz pairs;
4. $\mathcal{RP} \leftarrow \mathcal{RP} \cup \{\text{set of new Ritz pairs}\}$;
5. $n_{\text{crp}} \leftarrow n_{\text{crp}} + n_c$;
6. $v_{\text{init}} \leftarrow v_{k+1}$ from `getrtzp`.
7. For $i = 1, \dots, \rho_0$
8. use `getrtzp` to compute n_c Ritz pairs;
9. if necessary, swap new Ritz pair(s) with pair(s) in \mathcal{RP} .

Figure 5.1: Top: the basic algorithm `getrtzp` for computing Ritz pairs of $A^T A$. Bottom: the complete Lanczos algorithm `lsvdrr`, in which $e = (1, \dots, 1)^T$, \mathcal{RP} is the set of converged Ritz pairs, and n_{crp} is the total number of converged Ritz pairs.

because there is no guarantee that the Ritz values converge in the “natural order.” From Theorem 9.1.2 in [8], we know that the error $\sigma_j^2 - \theta_i^{(k)}$ in the i th Ritz value is bounded above as

$$|\sigma_j^2 - \theta_i^{(k)}| \leq |\beta_k s_{ki}|, \quad i = 1, \dots, k,$$

where β_k is the bottom off-diagonal element of T_k , and s_{ki} is the i th element of the bottom row of S_k . If we write $(\theta_i^{(k)})^{1/2} = \tilde{\sigma}_j^{(k)} = \sigma_j + \delta_j^{(k)}$, then

$$|\sigma_j^2 - \theta_i^{(k)}| = |\sigma_j + \tilde{\sigma}_j^{(k)}| |\sigma_j - \tilde{\sigma}_j^{(k)}| = |2\tilde{\sigma}_j^{(k)} - \delta_j^{(k)}| |\delta_j^{(k)}| \approx 2\tilde{\sigma}_j^{(k)} |\delta_j^{(k)}|,$$

showing that the quantity

$$e_i^{(k)} = |\beta_k s_{ki}| (\theta_i^{(k)})^{-1/2}, \quad i = 1, \dots, k \quad (5.1)$$

provides an estimate of the error in $\tilde{\sigma}_i^{(k)} = (\theta_i^{(k)})^{1/2}$ considered as an approximation to a singular value σ_j of A . Our criterion for accepting a Ritz value as converged is therefore

$$e_i^{(k)} < \tau \sigma_{\max}, \quad (5.2)$$

where τ is a user-specified tolerance, and σ_{\max} is an estimate of the largest singular value σ_1 .

From Thm. 8.1.2 in [8] we also know that if $\tilde{v}_i^{(k)}$ is the approximate eigenvector associated with $\theta_i^{(k)}$ then

$$\|A^T A \tilde{v}_i^{(k)} - \theta_i^{(k)} \tilde{v}_i^{(k)}\| = |\beta_k x_{ki}| = e_i^{(k)} \tilde{\sigma}_i^{(k)},$$

showing that small error estimates $e_i^{(k)}$ guarantee small residuals. Furthermore, according to Thm. 11.7.2 in [19], small residuals imply a small subspace angle between the subspaces spanned by the exact and approximate eigenvectors.

Unfortunately, the number of Lanczos iterations needed to capture p singular values, within the accuracy estimates provided by (5.1), may exceed p by a large factor. The cure to this difficulty is to *restart* the Lanczos process with an initial vector that is orthogonal to the set of converged Ritz vectors. This is easily archived in our algorithm, where the Ritz vectors are explicitly saved.

Let n_{crp} denote the total number of converged Ritz pairs, and let ℓ_0 be a fixed number greater than p , chosen by the user. Each time the Lanczos process is (re)started, we perform ℓ iterations. In our algorithm, one can either choose $\ell = \ell_0$ or $\ell = \ell_0 - n_{\text{crp}}$. The latter choice, which is default, ensures that a total of ℓ_0 Lanczos vectors are used.

When we have reached a stage where $n_{\text{crp}} = p$ Ritz values $\theta_i^{(k)}$ have converged according to (5.2), there is no guarantee that we have computed approximations to the desired p largest singular values. Our heuristic remedy for this difficulty is to restart the Lanczos process additional ρ_0 times, where ρ_0 is a small number (the default is $\rho_0 = 2$). Experiments in [6] show that these additional restarts indeed improve the reliability of the algorithm, at little extra cost.

Upon completion our algorithm `lsvdrr` returns approximations $\tilde{\sigma}_i$ and \tilde{v}_i to the largest p singular values and corresponding right singular vectors. Approximations to the left singular vectors can then be computed as $\tilde{u}_i = A\tilde{v}_i/\tilde{\sigma}_i$, and we emphasize that these vectors are not orthonormal. If an SVD routine is available, one can instead compute a diagonal matrix $\widehat{\Sigma}$ and two matrices \widehat{U} and \widehat{V} with orthonormal columns satisfying $A\widehat{V} = \widehat{U}\widehat{\Sigma}$, by means of the following procedure:

1. $A(\tilde{v}_1, \dots, \tilde{v}_p) = \hat{U} \hat{\Sigma} \hat{V}^T$ (SVD computation),
2. $\hat{V} \leftarrow (\tilde{v}_1, \dots, \tilde{v}_p) \hat{V}$.

More details about this approach can be found in [6], which also includes numerical results concerning the accuracy and efficiency of the `lsdrr` algorithm.

6. NUMERICAL EXAMPLES

We conclude with three demonstrations of the use of our package. The first example is available in the script `vsviddemo`, and shows how the three routines `hvsvid_L`, `hvsvid_R` and `lvsvd` can be used to compute symmetric indefinite VSV decompositions (2.1) of rank deficient KKT matrices of the form

$$A = \begin{pmatrix} M & N^T \\ N & 0 \end{pmatrix}.$$

In our test problems, M is an $m \times m$ symmetric semidefinite and rank-deficient matrix, and $N = \Theta M$ with Θ a $q \times m$ random matrix. The resulting matrix A has dimension $n = m + q$, and it is rank deficient and symmetric indefinite.

We generate 500 test matrices, and for each matrix and each VSV decomposition we compute the numerical rank r , the backward error $\|A - VT^T \Omega TV^T\|$, and the subspace angle between the numerical null space (spanned by the last $n - r$ singular vectors of A) and the approximate null space spanned by the last $n - r$ columns of V . A typical example of the results from such a test is shown in Fig. 6.1 for $m = 12$ and $q = 2$. Occasionally, the errors are in the range 10^{-13} – 10^{-9} , while most of the errors are less than 10^{-13} .

The second test problem is available in the function `ullivdemo` and illustrates the use of the ULLIV decomposition is noise and interference reduction. We generate a clean signal $s \in \mathbb{R}^N$ of length $N = 350$ consisting of a sum of 9 sinusoids with unit amplitude; see the DFT spectrum in the top of Fig. 6.2. The noisy signal is generated by adding white noise and an interfering signal to the clean signal; the white noise is generated by the Matlab command `0.5*randn(N,1)`, and the interfering signal is a sum of 16 sinusoids with amplitude 0.2. The DFT spectrum of the noisy signal is shown in the middle of Fig.6.2.

The filtered signal is then computed by means of the subspace method described in [12]. This involves the computation of the ULLIV decomposition (4.1) of two Hankel matrices A and B , the first being 311×40 and consisting of the noisy signal, and the second being 32×40 and representing the signal subspace of the interfering signal. From the ULLIV decomposition and the numerical rank p we then construct the matrix

$$X = U_A \Psi L_A \begin{pmatrix} L & 0 \\ 0 & I \end{pmatrix} V^T, \quad \Psi = \text{diag}(I_p, 0).$$

Finally we construct the filtered signal by averaging along the antidiagonals of X . The DFT spectrum of the filtered signal is shown in the bottom of Fig.6.2, and we see that we have indeed reduced the interference while maintaining most of the clean signal.

In the third test problem, which is available in the script `lsvdrrdemo`, we compute the k largest singular values and right singular vectors of a complex Toeplitz matrix of size 513×512 constructed from an NMR signal available as Data Set 002 at the BioSource database [1] of MRS signals. See, e.g., [22] for an application of such computations. The computations are performed for $k = 5, 10, 15$ and 20 , and for each k we compare the errors in the singular values and vectors, as well as the computing times, with those of the Matlab function `svds`.

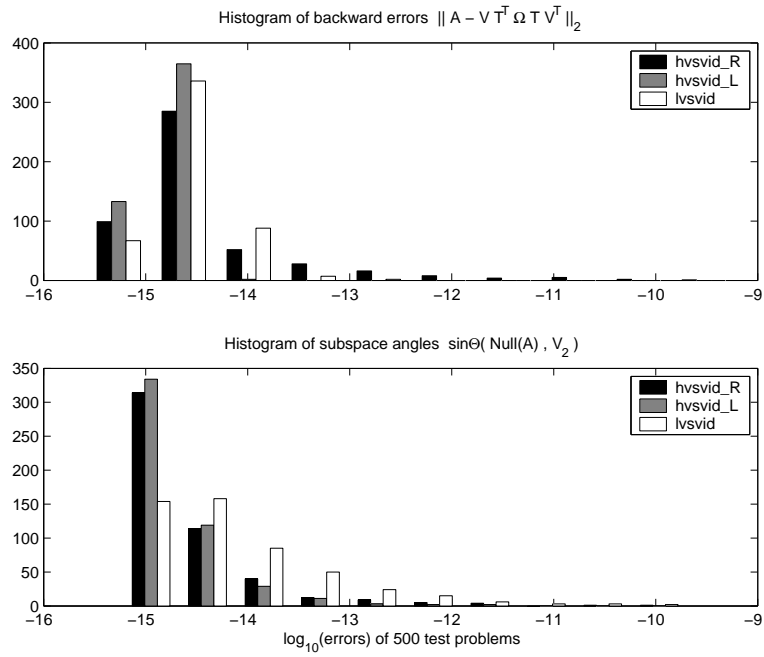


Figure 6.1: Backward errors and subspace angles for 500 KKT test problems of dimension 14×14 .

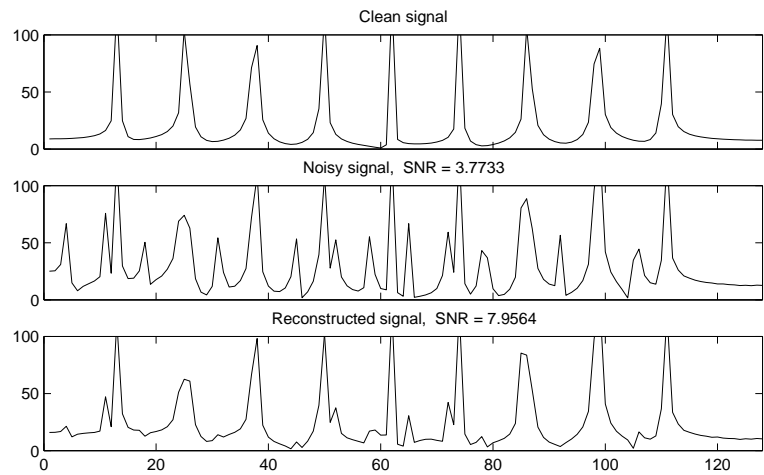


Figure 6.2: DFT spectra of the clean, noisy and filtered signals in ullivdemo test problem.

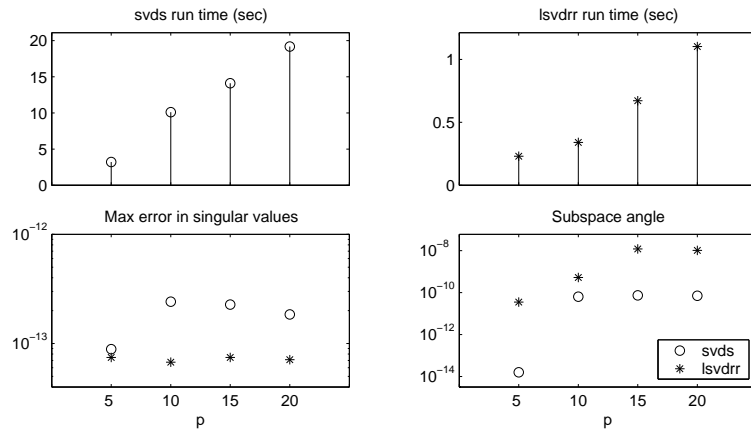


Figure 6.3: Computing times and errors for the largest k singular values and right singular vectors, computed by means of our Lanczos algorithm `lsvdrr` as well as Matlab's Lanczos algorithm implemented in the `svds` function. The bottom left figure reports $\max |\sigma_i - \tilde{\sigma}_i|$, $i = 1, \dots, p$, while the bottom right figure reports the subspace angle between the subspaces spanned by the dominant p right singular vectors and the approximations $\tilde{v}_1, \dots, \tilde{v}_p$.

We used the tolerance $\tau = 10^{-10}$ in the convergence criterion (5.2), and the matrix-vector multiplications with the Toeplitz matrix are done via Matlab's `fft` function. Figure 6.3 shows that for this test problem (using a 1.4 GHz Pentium), `lsvdrr` computes accurate singular values and right singular vectors faster than the general-purpose Lanczos routine `svds`. For comparison, Matlab's dense SVD routine computed all the singular values and right singular vectors in 8.5 seconds.

BIBLIOGRAPHY

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<http://www.esat.kuleuven.ac.be/sista/members/biomed/data002.htm>.
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7. OVERVIEW OF ROUTINES

| Demo Functions and Solvers | |
|-----------------------------------|--|
| lsvdrrdemo | Demonstrates the use of the restarted Lanczos algorithm implemented in <code>lsvdrr</code> and applied to NMR data from [1] |
| tvsv | Solves a symmetric num. rank-deficient system of equations |
| ullivdemo | Demonstrates the use of the high-rank ULLIV algorithm <code>ulliv</code> , applied to noise and interference reduction |
| vsviddemo | Demonstrates the use of the indefinite VSV algorithms <code>hvsvid_L</code> , <code>hvsvid_R</code> and <code>lvsvd</code> applied to symmetric indefinite KKT systems |

| Rank-Revealing Symmetric VSV Algorithms | |
|--|--|
| <code>hvsvid_L</code> | High-rank algorithm for indefinite matrix, L version |
| <code>hvsvid_R</code> | High-rank algorithm for indefinite matrix, R version |
| <code>hvsvd</code> | High-rank algorithm for semidefinite matrix |
| <code>lvsvd</code> | Low-rank algorithm for indefinite matrix |
| <code>lvsvd</code> | Low-rank algorithm for semidefinite matrix |
| <code>vsv_qrit</code> | Block QR refinement of VSV decomposition |

| VSV Up- and Downdating | |
|-------------------------------|---|
| <code>vsvd_L_mod</code> | Rank-one modification of indefinite matrix, L version |
| <code>vsvd_R_mod</code> | Rank-one modification of indefinite matrix, R version |
| <code>vsvd_up</code> | Rank-one update of semidefinite matrix |

| QLP Algorithms | |
|-----------------------|---|
| <code>hqlp</code> | High-rank gap-revealing QLP factorization |
| <code>lqlp</code> | QLP matrix approximation of a low-rank matrix |

| ULLIV Algorithms for a Matrix Pair (A, B) | |
|---|---|
| <code>ulliv</code> | Rank-revealing ULLIV decomposition, B has full row rank |
| <code>ulliv_up_A</code> | Rank-one update of the A matrix |
| <code>ulliv_up_B</code> | Rank-one update of the B matrix (rank increases) |

| Lanczos Algorithm with Reorthogonalization and Restarts | |
|--|---|
| <code>getrtzp</code> | Computation of Ritz pairs |
| <code>lsvdrr</code> | Driver routine for Lanczos algorithm |
| <code>tprod</code> | Toeplitz matrix-vector multiplication using FFT |
| <code>tprodinit</code> | Initialization routine for <code>tprod</code> |

| Misc. Tools | |
|--------------------|--|
| agl5 | Ashcraft-Grimes-Lewis 5×5 test matrix for LDL^T factorization |
| app_hyp | Apply a stabilized hyperbolic rotation |
| app_qrot | Apply a quadratic rotation |
| csi-10-10 | Mat-file with NMR data for lsvdrrdemo |
| gen_hyp | Generate a stabilized hyperbolic rotation |
| gen_qrot | Generate a quadratic rotation |
| hvsvd_cdef | Column deflation of upper triang. matrix in indef. VSV decomp. |
| hvsvd_rdef | Row deflation of lower triang. matrix in indef. VSV decomp. |
| lvsvd_cdef | Column deflation of lower triang. matrix in indef. VSV decomp. |
| TOTinviter | Inverse iterations applied to $T^T \Omega T$ |
| TOTlanczos | Lanczos method applied to $T^T \Omega T$ |
| TOTpowiter | Power iterations applied to $T^T \Omega T$ |
| vsvd_ip | Interim processor for indefinite VSV decomposition |

| | |
|--|--|
| Two routines from the Matrix Computation Toolbox [14] | |
|--|--|

| | |
|-----------|---|
| cholp | Pivoted Cholesky factorization |
| ldlt_symm | LDL^T factorization with symmetric or rook pivoting |

agl5

Purpose

Ashcraft-Grimes-Lewis 5-times-5 test problem for LDL^T factorization

Synopsis

[A,L,D] = agl5

Description

Generates a 5-times-5 test problem for the LDL^T factorization, such that L has a large entry when partial pivoting (Bunch-Kaufman) is used.

References

- [1] C. Ashcraft, R.G. Grimes and J.G. Lewis, "Accurate symmetric indefinite linear equation solvers," SIAM J. Matrix Anal. Appl., 20 (1999), pp. 513-561.

app_hyp

Purpose

Apply a stabilized hyperbolic rotation (left/right).

Synopsis

`[u1,u2] = app_hyp(v1,v2,c,s,sgn)`

Description

Apply a stabilized hyperbolic rotation, defined by the parameters c and s , from the left to the row vectors $v1$ and $v2$ such that

$$\begin{bmatrix} u1 \\ u2 \end{bmatrix} = \begin{bmatrix} ch & -sh \\ -sh & ch \end{bmatrix} \begin{bmatrix} v1 \\ v2 \end{bmatrix}$$

or from the right to the column vectors $v1$ and $v2$ such that

$$\begin{bmatrix} u1 & u2 \end{bmatrix} = \begin{bmatrix} v1 & v2 \end{bmatrix} \begin{bmatrix} ch & -sh \\ -sh & ch \end{bmatrix}$$

where $ch = 1/s$ and $sh = c/s$.

See Also

`gen_hyp` – Determine a 2-by-2 stabilized hyperbolic rotation.

References

- [1] S.T. Alexander, C.-T. Pan & R.J. Plemmons, “Analysis of recursive least squares hyperbolic rotation algorithms for signal processing,” *Lin. Alg. Appl.* 98 (1998), 3-40.

app_qrot

Purpose

Apply a quadratic rotation (left/right).

Synopsis

`[u1,u2,dd1,dd2] = app_qrot(v1,v2,c,s,d1,d2,sgn)`

Description

Apply a quadratic rotation H , defined by the parameters c and s , from the left to the row vectors $v1$ and $v2$ such that

$$\begin{bmatrix} u1 \\ u2 \end{bmatrix} = H \begin{bmatrix} v1 \\ v2 \end{bmatrix}$$

or from the right to the column vectors $v1$ and $v2$ such that

$$\begin{bmatrix} u1 & u2 \end{bmatrix} = \begin{bmatrix} u1 & u2 \end{bmatrix} H'$$

Also update the signature matrix:

$$\begin{bmatrix} dd1 & 0 \\ 0 & dd2 \end{bmatrix} = \text{sgn} * \begin{bmatrix} d1 & 0 \\ 0 & d2 \end{bmatrix}$$

where sgn is determined by the rotation.

See Also

`gen_qrot` – Determine a 2-by-2 quadratic rotation.

gen_hyp

Purpose

Determine a 2-by-2 stabilized hyperbolic rotation matrix.

Synopsis

`[c,s,r,sgn] = gen_hyp(a,b)`

Description

Compute a stabilized hyperbolic rotation to annihilate b using a, i.e., compute parameters c, s, and r such that

$$\begin{bmatrix} \text{ch} & -\text{sh} \\ -\text{sh} & \text{ch} \end{bmatrix} \begin{bmatrix} \text{a} \\ \text{b} \end{bmatrix} = \begin{bmatrix} \text{r} \\ 0 \end{bmatrix} \quad \text{with} \quad \begin{bmatrix} \text{ch} & -\text{sh} \\ -\text{sh} & \text{ch} \end{bmatrix} \text{S} \begin{bmatrix} \text{ch} & -\text{sh} \\ -\text{sh} & \text{ch} \end{bmatrix} = \text{sgn} * \text{S}$$

where $\text{ch} = 1/s$ and $\text{sh} = c/s$, and where the signature matrix S is either

$$\text{S} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{or} \quad \text{S} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} .$$

See Also

`app_hyp` – Apply a stabilized hyperbolic rotation.

References

- [1] S.T. Alexander, C.-T. Pan & R.J. Plemmons, “Analysis of recursive least squares hyperbolic rotation algorithms for signal processing,” *Lin. Alg. Appl.* 98 (1998), 3-40.

gen_qrot

Purpose

Determine a 2-by-2 quadratic rotation matrix.

Synopsis

`[c,s,r,sgn] = gen_qrot(a,b,d1,d2)`

Description

Compute a real quadratic (Givens or hyperbolic) rotation H to annihilate b using a , i.e., compute c , s , and r such that

$$H \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix} \quad \text{with} \quad H' S H = \text{sgn} * S$$

where the signature matrix S is

$$S = \begin{bmatrix} d1 & 0 \\ 0 & d2 \end{bmatrix}, \quad d1, d2 = +1, -1.$$

See Also

`app_qrot` – Apply a quadratic rotation.

getrtzp

Purpose

Compute (additional) Ritz pairs for a cross-product matrix

Synopsis

```
[rtzvals,rtzvecs,errests,nconv,num_iter,vnext,smax] = ...  
getrtzp(A,k,ncrp,Vk,max_iter,vinit,tol,smax)
```

Description

Applies Lanczos iterations to the matrix A^*A ; the Lanczos vectors are explicitly re-orthogonalized internally, as well as with respect to an existing set of converged vectors. A singular value estimate is considered as converged when an error estimate is below $smax*tol$.

Input Parameters

| | |
|----------|---|
| A | matrix; |
| k | number of desired singular values; |
| ncrp | number of converged Ritz pairs so far; |
| Vk | previously converged Ritz vectors; |
| max_iter | max. no. of Lanczos iterations in this call to getrtzp; |
| vinit | start vector; |
| tol | relative residual tolerance; |
| smax | current estimate of largest singular value; |

Output Parameters

| | |
|----------|---|
| rtzvals | converged Ritz values of A^*A ; |
| rtzvecs | corresponding converged Ritz vectors; |
| errests | corresponding error estimates of singular values; |
| nconv | number of converged Ritz pairs; |
| num_iter | number of iterations used in the call to getrtzp; |
| vnext | vector for next call to getrtzp; |
| smax | updated value of smax; |

References

- [1] R.D. Fierro and E.P. Jiang, "Lanczos and the Riemannian SVD in information retrieval applications," Numer. Lin. Alg. Appl., to appear.

hqlp

Purpose

High-rank gap-revealing QLP factorization.

Synopsis

```
[p,L,P,Q] = hqlp(A)
[p,L,P,Q] = hqlp(A,gap_tol)
```

Description

Computes a gap-revealing factorization $A = Q*L*P'$, in which Q and P are orthogonal matrices, and L is a lower triangular matrix whose diagonal elements sometimes approximate the singular values of A . Also returns the largest p such that $\text{abs}(L(p,p)/L(p+1,p+1)) > \text{gap_tol}$. Designed for high-rank matrices; use `lqlp` for low-rank matrices.

Input Parameters

| | |
|----------------------|---|
| <code>A</code> | general matrix; |
| <code>gap_tol</code> | tolerance for gap detection; |
| Defaults | <code>gap_tol = min(size(A))/eps</code> ; |

Output Parameters

| | |
|----------------|---|
| <code>p</code> | estimate of numerical rank of A ; |
| <code>L</code> | lower triangular matrix in $A = Q*L*P'$; |
| <code>P</code> | right orthogonal matrix; |
| <code>Q</code> | left orthogonal matrix; |

Algorithm

A pivoted QR factorization $A*Pi_p = Q*R$ is followed by a pivoted QR factorization $R'*Pi_q = P*L'$; thus $A = (Q*Pi_q)*L*(Pi_p*P)'$. The diagonal elements of L sometimes track the singular values of A , but this is not guaranteed; hence the factorization cannot be guaranteed to reveal rank.

See Also

`lqlp` – pivoted QLP matrix approximation with interleaved factorizations.

References

- [1] G.W. Stewart, "The QLP approximation to the singular value decomposition," *SIAM J. Sci. Comp.*, 20 (1999), pp. 1336-1348.

hvsvid_L

Purpose

High-rank revealing decomp. of a sym. indef. matrix, L version.

Synopsis

```
[p,L,Omega,V] = hvsvid_L(A)
[p,L,Omega,V] = hvsvid_L(A,tol_rank)
[p,L,Omega,V] = hvsvid_L(A,tol_rank,max_iter)
[p,L,Omega,V] = hvsvid_L(A,tol_rank,max_iter,fixed_rank)
```

Description

Computes a rank-revealing VSV decomposition $A = V*(L'*Omega*L)*V'$ of a symmetric indefinite n-by-n matrix. Only the upper triangular part needs to be specified. Optimized for matrices whose rank p close to n. Function hvsvid_R computes the R version.

Input Parameters

| | |
|------------|---|
| A | symmetric indefinite matrix; |
| tol_rank | rank decision tolerance; |
| max_iter | max. number of inverse iterations per deflation step, used in the singular vector estimator; |
| fixed_rank | deflate to the fixed rank given by fixed_rank instead of using the rank decision tolerance; |
| Defaults | tol_rank = n*norm(A,1)*eps; max_iter = 5; |

Output Parameters

| | |
|-------|--|
| p | numerical rank of A; |
| L | lower triangular matrix in $A = V*(L'*Omega*L)*V'$; |
| Omega | signature matrix in $A = V*(L'*Omega*L)*V'$; |
| V | orthogonal matrix in $A = V*(L'*Omega*L)*V'$; |

Algorithm

The symmetric indefinite matrix A is preprocessed by a pivoted LDL' factorization. An interim stage (where D is made diagonal) is followed by a rank-revealing ULV-like decomposition, using inverse iterations for singular vector estimation.

See Also

| | |
|----------|--|
| hvsvid_R | – High-rank revealing VSV alg. for sym. indef. matrices, R version |
| hvsvid | – High-rank revealing VSV alg. for symmetric semidefinite matrices |
| lvsvd | – Low-rank revealing VSV alg. for symmetric indefinite matrices |
| lvsvd | – Low-rank revealing VSV alg. for symmetric semidefinite matrices |

References

- [1] P.C. Hansen & P.Y. Yalamov, "Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization", *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443-458.

hvsvid_R

Purpose

High-rank revealing decomp. of a sym. indef. matrix, R version.

Synopsis

```
[p,R,Omega,V] = hvsvid_R(A)
[p,R,Omega,V] = hvsvid_R(A,tol_rank)
[p,R,Omega,V] = hvsvid_R(A,tol_rank,max_iter)
[p,R,Omega,V] = hvsvid_R(A,tol_rank,max_iter,fixed_rank)
```

Description

Computes a rank-revealing VSV decomposition $A = V*(R'*Omega*R)*V'$ of a symmetric indefinite n-by-n matrix. Only the upper triangular part needs to be specified. Optimized for matrices whose rank p is close to n. Functions hvsvid and lvsvid compute the L-version of the decomposition.

Input Parameters

| | |
|------------|---|
| A | symmetric indefinite matrix; |
| tol_rank | rank decision tolerance; |
| max_iter | max. number of inverse iterations per deflation step, used in the singular vector estimator; |
| fixed_rank | deflate to the fixed rank given by fixed_rank instead of using the rank decision tolerance; |
| Defaults | tol_rank = n*norm(A,1)*eps; max_iter = 5; |

Output Parameters

| | |
|-------|--|
| p | numerical rank of A; |
| R | upper triangular matrix in $A = V*(R'*Omega*R)*V'$; |
| Omega | signature matrix in $A = V*(R'*Omega*R)*V'$; |
| V | orthogonal matrix in $A = V*(R'*Omega*R)*V'$; |

Algorithm

The symmetric indefinite matrix A is preprocessed by a pivoted LDL' factorization. An interim stage (where D is made diagonal) is followed by a rank-revealing URV-like decomposition, using inverse iterations for singular vector estimation.

See Also

| | |
|----------|--|
| hvsvid_L | – High-rank revealing VSV alg. for sym. indef. matrices, L version |
| hvsvid | – High-rank revealing VSV alg. for symmetric semidefinite matrices |
| lvsvid | – Low-rank revealing VSV alg. for symmetric indefinite matrices |
| lvsvid | – Low-rank revealing VSV alg. for symmetric semidefinite matrices |

References

- [1] P.C. Hansen & P.Y. Yalamov, "Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization", *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443-458.

hvsvid_cdef

Purpose

Deflate one column of R in the high-rank URV-like VSV algorithm.

Synopsis

$[R, \Omega, V, \text{fail}] = \text{hvsvid_cdef}(R, \Omega, V, r, \text{vmin})$

Description

Given the decomposition $V \cdot R' \cdot \Omega \cdot R \cdot V'$, the function deflates the last column of $R(1:r, 1:r)$. vmin is an estimate of the right singular vector of $R(1:r, 1:r)' \cdot \Omega(1:r, 1:r) \cdot R(1:r, 1:r)$ associated with the smallest singular value sigma_r . On return, the norm of the last column of $R(1:r, 1:r)' \cdot \Omega(1:r, 1:r) \cdot R(1:r, 1:r)$ is of the order sigma_r . The matrix V can be left out by inserting an empty matrix $[]$.

Input Parameters

| | |
|---------------|---|
| R | upper triangular matrix in $A = V \cdot (R' \cdot \Omega \cdot R) \cdot V'$; |
| Ω | signature matrix in $A = V \cdot (R' \cdot \Omega \cdot R) \cdot V'$; |
| V | orthogonal matrix in $A = V \cdot (R' \cdot \Omega \cdot R) \cdot V'$; |
| r | size of submatrix to be deflated; |
| vmin | estimate of the smallest right singular vector of the product $R(1:r, 1:r)' \cdot \Omega(1:r, 1:r) \cdot R(1:r, 1:r)$; |

Output Parameters

| | |
|---------------|---|
| R | upper triangular matrix in resulting $A = V \cdot (R' \cdot \Omega \cdot R) \cdot V'$; |
| Ω | signature matrix in resulting $A = V \cdot (R' \cdot \Omega \cdot R) \cdot V'$; |
| V | orthogonal matrix in resulting $A = V \cdot (R' \cdot \Omega \cdot R) \cdot V'$; |
| fail | true if a hypernormal rotation is ill defined; |

References

- [1] P.C. Hansen & P.Y. Yalamov, "Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization", *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443-458.

hvsvid_rdef

Purpose

Deflate one row of L in the high-rank ULV-like VSV algorithm.

Synopsis

$[L,V,\Omega] = \text{hvsvid_rdef}(L,V,\Omega,r,vmin)$

Description

Given the decomposition $V*L'*\Omega*L*V'$, the function deflates the last row of $L(1:r,1:r)$. $vmin$ is an estimate of the right singular vector of $L(1:r,1:r)*\Omega(1:r,1:r)*L(1:r,1:r)$ associated with the smallest singular value $\sigma_{a,r}$. On return, the norm of the last column of $L(1:r,1:r)*\Omega(1:r,1:r)*L(1:r,1:r)$ is of the order $\sigma_{a,r}$. The matrix V can be left out by inserting an empty matrix $[]$.

Input Parameters

| | |
|----------|---|
| L | lower triangular matrix in $A = V*(L'*\Omega*L)*V'$; |
| Ω | signature matrix in $A = V*(L'*\Omega*L)*V'$; |
| V | orthogonal matrix in $A = V*(L'*\Omega*L)*V'$; |
| r | size of submatrix to be deflated; |
| $vmin$ | estimate of the smallest right singular vector of the product $L(1:r,1:r)*\Omega(1:r,1:r)*L(1:r,1:r)$; |

Output Parameters

| | |
|----------|---|
| L | upper triangular matrix in resulting $V*(L'*\Omega*L)*V'$; |
| V | orthogonal matrix in resulting $V*(L'*\Omega*L)*V'$; |
| Ω | signature matrix in resulting $V*(L'*\Omega*L)*V'$; |

References

- [1] P.C. Hansen & P.Y. Yalamov, "Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization", *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443-458.

hsvsd

Purpose

High-rank revealing decomposition of a symmetric semidefinite matrix.

Synopsis

```
[p,L,V] = hsvsd(A)
[p,L,V] = hsvsd(A,tol_rank)
[p,L,V] = hsvsd(A,tol_rank,fixed_rank)
```

Description

Computes a rank-revealing VSV decomposition $A = V*(L'*L)*V'$ of a symmetric semidefinite n -by- n matrix. Only the upper triangular part needs to be specified. Optimized for matrices whose rank p is close to n .

Input Parameters

| | |
|------------|---|
| A | symmetric semidefinite matrix; |
| tol_rank | rank decision tolerance; |
| fixed_rank | deflate to the fixed rank given by fixed_rank instead of using the rank decision tolerance; |
| Defaults | tol_rank = $n*\text{norm}(A,1)*\text{eps}$; |

Output Parameters

| | |
|---|--|
| p | numerical rank of A; |
| L | lower triangular matrix in $A = V*(L'*L)*V'$; |
| V | orthogonal matrix in $A = V*(L'*L)*V'$; |

Algorithm

The symmetric semidefinite matrix A is preprocessed by a pivoted Cholesky factorization and then postprocessed by a high-rank-revealing ULV decomposition. An indefinite matrix results in an error message during the Cholesky factorization.

See Also

| | |
|---------|--|
| hsvsd_L | – High-rank revealing VSV alg. for sym. indef. matrices, L version |
| hsvsd_R | – High-rank revealing VSV alg. for sym. indef. matrices, R version |
| lsvsd | – Low-rank revealing VSV alg. for symmetric indefinite matrices |
| lsvsd | – Low-rank revealing VSV alg. for symmetric semidefinite matrices |

References

- [1] P.C. Hansen & P.Y. Yalamov, “Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization”, *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.

lqlp

Purpose

Pivoted QLP matrix approximation with interleaved factorizations.

Synopsis

```
[p,L,P,Q,gap_ratio] = lqlp(A)
[p,L,P,Q,gap_ratio] = lqlp(A,tol_gap)
[p,L,P,Q,gap_ratio] = lqlp(A,tol_gap,fixed_rank)
```

Description

Computes a rank- p pivoted QLP matrix approximation of an m -by- n matrix A ($m \geq n$) satisfying $A*P = Q*L$ with a lower triangular p -by- p matrix L . The rank (or stopping point) p is either `fixed_rank` or is dynamically determined by `tol_gap`. The absolute value of the diagonal elements of L are approximations to the first p singular values of A , while the columns of Q and P approximate the first p left and right singular vectors of A .

Input Parameters

| | |
|-------------------------|--|
| <code>A</code> | m -by- n matrix ($m \geq n$); |
| <code>tol_gap</code> | truncate the decomposition after computing a rank- p approximation to A , where p is the smallest integer such that $\text{abs}(L(p,p)/L(p+1,p+1)) \geq \text{tol_gap}$; |
| <code>fixed_rank</code> | ignore <code>tol_gap</code> and truncate the decomposition after computing an approximation to A of rank <code>fixed_rank</code> . |
| Defaults | <code>tol_gap</code> = n/eps ; <code>fixed_rank</code> = n . |

Output Parameters

| | |
|------------------------|---|
| <code>p</code> | smallest integer such that $\text{abs}(L(p,p)/L(p+1,p+1)) < \text{tol_gap}$ (or <code>fixed_rank</code>); |
| <code>L</code> | p -by- p lower triangular matrix whose diagonal elements, in absolute value, track the largest p singular values of A ; |
| <code>P, Q</code> | matrices with p orthonormal columns; |
| <code>gap_ratio</code> | $\text{abs}(L(p+1,p+1)/L(p,p))$, that is, the ratio of the first approximate singular value excluded to the last one included, empty if $p = n$ or <code>fixed_rank</code> = n . |

Algorithm

The first p rows and columns of the pivoted QR factorization of A are computed, $A*P_{i-1} = Q*R$. Then the pivoted QR factorization of R' is computed, $R'*P_{i-2} = P*L'$, where L' is p -by- p . The rank p is either `fixed_rank` or is determined dynamically by the following. The computation of R is stopped after k_1 rows and columns, where $\text{abs}(R(k_1,k_1)/R(k_1-1,k_1-1)) \leq \text{tol_gap}$. Then rows and columns of L' are computed to see whether $\text{abs}(L(j,j)/L(j-1,j-1)) \leq \text{tol_gap}$ for any $j \leq k_1$. If so, the algorithm halts after computing these j rows and columns of L , and the final approximation to the SVD of A is rank j . If not, the next k_2 rows and columns of R are computed until `tol_gap` is achieved, then corresponding rows and columns of L ($k_1 + j$, $1 \leq j \leq k_2$) are computed to see whether `tol_gap` holds at any j and the computation can be halted. If not, more rows and columns of R are computed, etc. This process is called interleaving.

See Also

hqlp – high-rank gap-revealing QLP factorization.

References

- [1] G.W. Stewart, “The QLP approximation to the singular value decomposition,” *SIAM J. Sci. Comp.*, 20 (1999), pp. 1336-1348.
- [2] D.A. Huckaby and T.F. Chan, “Stewart’s pivoted QLP decomposition for low-rank matrices,” Tech. Report CAM-02-54, Dept. Mathematics, UCLA, 2002.

lsvdr

Purpose

Lanczos SVD with reorthogonalization and explicit restarts

Synopsis

```
[sk,Vk,nits,nrst,errests] = lsvdr(A,k,max_iter,max_restarts,conserve,safety)
```

Description

Computes approximations to the k dominant singular triplets, using the Lanczos method with reorthogonalization and explicit restarts. The stopping criterion is that the error in each computed singular value must be smaller than tol times the largest singular value.

Input Parameters

| | |
|--------------|--|
| A | dense/sparse matrix or structure with Toeplitz matrix; |
| k | number of desired singular triplets; |
| tol | tolerance for relative residual of triplets; |
| max_iter | maximum number of Lanczos iterations per restart; |
| max_restarts | maximum number of Lanczos restarts; |
| conserve | if 1 then max_iter Lanczos vectors are used in total, otherwise max_iter vectors are used in each restart; |
| safety | perform additional safety restarts, after k Ritz values have converged; |
| Defaults | tol = 1e-4; max_iter = min(2*k,n) max_restarts = 100; conserve = 1; safety = 2; |

Output Parameters

| | |
|---------|---|
| sk | vector of singular value estimates; |
| Vk | matrix of right singular vector approximations; |
| nits | number of times A and A' combined have been referenced; |
| nrst | number of restarts; |
| errests | vector of error estimates for singular values; |

Matrix Representation

The input parameter A can be either a matrix (dense or sparse) or a structure that holds information about a Toeplitz matrix: A.col = first column of A, A.row = first row of A.

References

- [1] R.D. Fierro and E.P. Jiang, "Lanczos and the Riemannian SVD in information retrieval applications," Numer. Lin. Alg. Appl., to appear.

lvsvd

Purpose

Low-rank revealing decomposition of a symmetric indefinite matrix.

Synopsis

```
[p,L,Omega,V] = lvsvd(A)
[p,L,Omega,V] = lvsvd(A,tol_rank)
[p,L,Omega,V] = lvsvd(A,tol_rank,max_iter)
[p,L,Omega,V] = lvsvd(A,tol_rank,max_iter,est_type)
[p,L,Omega,V] = lvsvd(A,tol_rank,max_iter,est_type,fixed_rank)
```

Description

Computes a rank-revealing VSV decomposition $A = V*(R'*Omega*R)*V'$ of a symmetric indefinite n -by- n matrix. Only the upper triangular part needs to be specified. Optimized for matrices whose rank p is small compared to n .

Input Parameters

| | |
|------------|--|
| A | symmetric indefinite matrix; |
| tol_rank | rank decision tolerance; |
| max_iter | max. number of power/Lanczos iterations per deflation step, used in the singular vector estimator; |
| est_type | if true, then estimate singular vectors by means of the Lanczos procedure, else use the power method; |
| fixed_rank | deflate to the fixed rank given by fixed_rank instead of using the rank decision tolerance; |
| Defaults | tol_rank = $n*\text{norm}(A,1)*\text{eps}$; max_iter = 5; est_type = 0 (power method); |

Output Parameters

| | |
|-------|--|
| p | numerical rank of A; |
| L | lower triangular matrix in $A = V*(L'*Omega*L)*V'$; |
| Omega | signature matrix in $A = V*(L'*Omega*L)*V'$; |
| V | orthogonal matrix in $A = V*(L'*Omega*L)*V'$; |

See Also

| | |
|----------|--|
| hsvsvd | – High-rank revealing VSV alg. for symmetric indefinite matrices |
| hsvsvd_R | – High-rank revealing VSV alg., sym. indef. matrices, R version |
| hsvsvd | – High-rank revealing VSV alg. for symmetric semidefinite matrices |
| lvsvd | – Low-rank revealing VSV alg. for symmetric semidefinite matrices |

References

- [1] P.C. Hansen & P.Y. Yalamov, “Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization”, *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.

lvsvd_cdef

Purpose

Deflate one column of L in the low-rank ULV-like VSV algorithm.

Synopsis

$[L, \Omega, V] = \text{lvsvd_cdef}(L, \Omega, V, r, v_{\max})$

Description

Given the VSV decomposition $V * L' * \Omega * L * V'$, the function deflates the first column of $L(r:n, r:n)$. v_{\max} is an estimate of the right singular vector of $L(r:n, r:n)' * \Omega(r:n, r:n) * L(r:n, r:n)$ associated with the largest singular value σ_{\max} . On return, the norm of the first column of $L(r:n, r:n)' * \Omega(r:n, r:n) * L(r:n, r:n)$ is of the order σ_{\max} . The matrix V can be left out by inserting an empty matrix $[]$.

Input Parameters

L lower triangular matrix in $A = V * (L' * \Omega * L) * V'$;
Omega signature matrix in $A = V * (L' * \Omega * L) * V'$;
V orthogonal matrix in $A = V * (L' * \Omega * L) * V'$;
r size of submatrix to be deflated;
vmin estimate of the smallest right singular vector of
 the product $L(1:r, 1:r)' * \Omega(1:r, 1:r) * L(1:r, 1:r)$;

Output Parameters

L lower triangular matrix in resulting $A = V * (L' * \Omega * L) * V'$;
Omega signature matrix in resulting $A = V * (L' * \Omega * L) * V'$;
V orthogonal matrix in resulting $A = V * (L' * \Omega * L) * V'$;
V orthogonal matrix in resulting $A = V * (L' * \Omega * L) * V'$;

References

- [1] R.D. Fierro and P.C. Hansen, "Low-Rank Revealing UTV Decompositions", Numerical Algorithms, 15 (1997), pp. 37–55.

lsvsd

Purpose

Low-rank revealing decomposition of a symmetric semidefinite matrix.

Synopsis

```
[p,L,V] = lsvsd(A)
[p,L,V] = lsvsd(A,tol_rank)
[p,L,V] = lsvsd(A,tol_rank,max_iter)
[p,L,V] = lsvsd(A,tol_rank,max_iter,est_type)
[p,L,V] = lsvsd(A,tol_rank,max_iter,est_type,fixed_rank)
```

Description

Computes a rank-revealing VSV decomposition $A = V*(L'*L)*V'$ of a symmetric semidefinite n -by- n matrix. Only the upper triangular part of needs to be specified. Optimized for matrices whose rank p is small compared to n .

Input Parameters

| | |
|------------|---|
| A | symmetric semidefinite matrix; |
| tol_rank | rank decision tolerance; |
| max_iter | max. number of inverse iterations per deflation step, used in the singular vector estimator; |
| est_type | if true, then estimate singular vectors by means of the Lanczos procedure, else use the power method; |
| fixed_rank | deflate to the fixed rank given by fixed_rank instead of using the rank decision tolerance; |
| Defaults | tol_rank = $n*\text{norm}(A,1)*\text{eps}$; max_iter = 5; est_type = 0 (power method); |

Output Parameters

| | |
|---|--|
| p | numerical rank of A; |
| L | lower triangular matrix in $A = V*(L'*L)*V'$; |
| V | orthogonal matrix in $A = V*(L'*L)*V'$; |

Algorithm

The symmetric semidefinite matrix A is preprocessed by a pivoted Cholesky factorization and then postprocessed by a low-rank revealing ULV decomposition, using either power or Lanczos iterations to estimate the dominant singular vectors. An indefinite matrix results in an error message during the Cholesky factorization.

See Also

| | |
|----------|--|
| hvsvid | – High-rank revealing VSV alg. for symmetric indefinite matrices |
| hvsvid_R | – High-rank revealing VSV alg., sym. indef. matrices, R version |
| hvsvd | – High-rank revealing VSV alg. for symmetric semidefinite matrices |
| lsvvid | – Low-rank revealing VSV alg. for symmetric indefinite matrices |

References

- [1] P.C. Hansen & P.Y. Yalamov, “Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization”, *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.

TOTinviter

Purpose

Inverse iterations for $T^* \Omega T$.

Synopsis

`[smin,vmin] = TOTinviter(T,Omega,itmax)`

Description

Inverse iterations on the product $T^* \Omega T$ to compute the smallest singular value and the corresponding singular vector.

Input Parameters

| | |
|-------|-------------------------------|
| T | triangular matrix; |
| Omega | diagonal matrix; |
| itmax | maximum number of iterations; |

Output Parameters

| | |
|------|--|
| smin | estimate of smallest singular value; |
| vmin | estimate of corresponding singular vector; |

TOTlanczos

Purpose

Symmetric Lanczos procedure for $T' * \Omega * T$.

Synopsis

[smax,vmax] = TOTlanczos(T,Omega,itmax)

[smax,vmax] = TOTlanczos(T,Omega,itmax,reorth)

Description

Computes an estimate of the largest singular value and the associated singular vector of the matrix $T' * \Omega * T$ using a maximum of itmax Lanczos iterations. If reorth = 1, then MGS reorthogonalization is used.

Input Parameters

| | |
|----------|-----------------------------------|
| T | matrix; |
| Omega | diagonal matrix; |
| itmax | maximum number of iterations; |
| reorth | MGS reorthogonalization if true; |
| Defaults | reorth = 1 (reorthogonalization). |

Output Parameters

| | |
|------|--|
| smin | estimate of smallest singular value; |
| vmin | estimate of corresponding singular vector; |

See Also

TOTpowiter – Power iterations for $T' * \Omega * T$

References

- [1] G.H. Golub and C.F. Van Loan, “Matrix Computations”, Johns Hopkins University Press, 3. Ed., 1996; p. 480.

TOTpowiter

Purpose

Power iterations for $T^* \Omega T$.

Synopsis

$[smin, vmin] = \text{TOTpowiter}(T, \Omega, itmax)$

Description

Power iterations on the product $T^* \Omega T$ to compute the largest singular value and the corresponding singular vector.

Input Parameters

| | |
|-------|-------------------------------|
| T | triangular matrix; |
| Omega | diagonal matrix; |
| itmax | maximum number of iterations; |

Output Parameters

| | |
|------|--|
| smin | estimate of largest singular value; |
| vmin | estimate of corresponding singular vector; |

See Also

TOTlanczos – Lanczos procedure for $T^* \Omega T$

tprod

Purpose

Toeplitz matrix-vector multiplication via FFT.

Synopsis

```
y = tprod(lambda,m,n,x,transp)
```

Description

This routine computes $T*x$ for `transp = 0` or $T'*x$ for `value = 1`, where T is an m -by- n Toeplitz matrix, using the eigenvalues `lambda` of a related circulant matrix computed by means of `tprodinit`.

Input Parameters

| | |
|---------------------|--|
| <code>lambda</code> | eigenvalue vector need for the FFT; |
| <code>m, n</code> | dimensions of Toeplitz matrix; |
| <code>x</code> | vector to be multiplied by T ; |
| <code>transp</code> | if 0 or nonexisting, multiply with T , ortherwise multiply with T' ; |

Output Parameters

| | |
|----------------|-----------------------|
| <code>y</code> | matrix-vector product |
|----------------|-----------------------|

Algorithm

Let `lambda` be the eigenvalues of a circulant matrix derived from T (see `tprodinit`); then the product $T*x$ consists of the first m elements of the vector `ifft(lambda.*fft([x,z]))`, where `z` is a vector of zeros, while the product $T'*x$ consists of the first n elements of the vector `ifft(conj(lambda).*fft([x,z]))`.

See Also

`tprodinit` – Initialization routine for `tprod`

References

- [1] P.C. Hansen, "Deconvolution and regularization with Toeplitz matrices," Numer. Algo. 29 (2002), pp. 323-378.

tprodinit

Purpose

Initialization routine for tprod (Toeplitz matrix-vector product)

Synopsis

```
lambda = tprodinit(colT,rowT)
```

Description

lambda contains the eigenvalues of a related circulant matrix, needed for matrix-vector multiplication with the Toeplitz matrix specified by colT and rowT. The length of lambda is a power of 2.

Input Parameters

colT contains the first column of the Toeplitz matrix;
rowT contains the first row of the Toeplitz matrix;

Output Parameters

lambda contains the eigenvalues of an extended circulant matrix;

Algorithm

lambda contains the eigenvalues of the circulant matrix C whose first column is $c = [\text{colT};z;\text{rowT}(\text{end}:-1:2)]$, where z is a zero columns with dimensions such that $\text{length}(c)$ is a power of 2 (for efficiency).

See Also

tprod – Toeplitz matrix-vector product, using tprodinit

References

- [1] P.C. Hansen, "Deconvolution and regularization with Toeplitz matrices," Numer. Algo. 29 (2002), pp. 323-378.

tvsv

Purpose

Solves a rank-deficient system using the VSV decomposition.

Synopsis

$x_{\text{tvsv}} = \text{tvsv}(L, V, p, b)$

$x_{\text{tvsv}} = \text{tvsv}(R, \Omega, V, p, b)$

$x_{\text{tvsv}} = \text{tvsv}(L, \Omega, V, p, b)$

Description

Solves the symmetric and near-rank deficient system of equations $Ax = b$, using the rank-revealing VSV decomposition of A . Three decompositions of A can be used:

$A = V * L' * L * V'$ (semidefinite A , lower triangular L)

$A = V * R' * \Omega * R * V'$ (indefinite A , upper triangular R)

$A = V * L' * \Omega * L * V'$ (indefinite A , lower triangular L)

Input Parameters

Semindefinite case:

L lower triangular matrix;

V orthogonal matrix;

p numerical rank;

b right-hand side;

Indefinite case:

L or R lower or upper triangular matrix;

Ω signature matrix

V orthogonal matrix;

p numerical rank;

b right-hand side;

Output Parameters

x_{tvsv} truncated VSV solution;

References

- [1] P. C. Hansen and P. Y. Yalamov, "Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization," *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.

ulliv

Purpose

High-rank-revealing ULLV algorithm, B full row rank.

Synopsis

[p,LA,L,V,UA,UB,vec] = ulliv(A,B)

[p,LA,L,V,UA,UB,vec] = ulliv(A,B,tol_rank)

[p,LA,L,V,UA,UB,vec] = ulliv(A,B,tol_rank,tol_ref,max_ref)

[p,LA,L,V,UA,UB,vec] = ulliv(A,B,tol_rank,tol_ref,max_ref,fixed_rank)

Description

Computes a rank-revealing ULLIV decomposition of an m_A -by- n matrix A with $m_A \geq n$, and an m_B -by- n matrix B with full row rank $m_B \leq n$:

$$A = UA*LA*[\begin{smallmatrix} L & 0 \\ 0 & I \end{smallmatrix}]*V' \quad \text{and} \quad B = UB*[\begin{smallmatrix} L & 0 \\ 0 & I \end{smallmatrix}]*V'$$

Here, LA is n -by- n and L is m_B -by- m_B and both are lower triangular; UA , UB and V are unitary matrices, where only the first n_A column of UA are computed.

The ULLV decomposition is a quotient ULV decomposition of the quotient $A*\text{pinv}(B)_A$, where $\text{pinv}(B)_A$ is the A -weighted pseudoinverse of B :

$$A*\text{pinv}(B)_A = UA(:,1:m_B)*LA(1:m_B,1:m_B)*UB' \quad .$$

Hence the lower triangular matrix $LA(1:m_B,1:m_B)$ reveals the numerical rank p of the matrix quotient.

Note that the algorithm is optimized for numerical rank p close to n_B , and that this algorithm should not be used if B is ill conditioned or rank deficient. Use the function `ullv` if B has full column rank.

Input Parameters

| | |
|-------------------|--|
| A | m_A -by- n matrix ($m_A \geq n$); |
| B | m_B -by- n matrix ($m_B \leq n$); |
| tol_rank | rank decision tolerance; |
| tol_ref | upper bound on the 2-norm of the off-diagonal block $LA(p+1:n,1:p)$ relative to the Frobenius-norm of LA ; |
| max_ref | max. number of refinement steps per singular value to achieve the upper bound <code>tol_ref</code> ; |
| fixed_rank | deflate to the fixed rank given by <code>fixed_rank</code> instead of using the rank decision tolerance; |
| Defaults | <code>tol_rank = sqrt(n)*norm(A,1)*eps;</code> <code>tol_ref = 1e-04;</code> <code>max_ref = 0;</code> |

Output Parameters

p numerical rank of $A \cdot \text{pinv}(B) \cdot A$;
 LA, L, V, UA, UB the ULLV factors;

vec a 5-by-1 vector with:
 $vec(1)$ = upper bound of $\text{norm}(LA(p+1:n, 1:p))$,
 $vec(2)$ = estimate of p th singular value,
 $vec(3)$ = estimate of $(p+1)$ th singular value,
 $vec(4)$ = a posteriori upper bound of num. nullspace angle,
 $vec(5)$ = a posteriori upper bound of num. range angle.

Algorithm

First compute the LQ factorization $B = [L, 0] \cdot V'$ and then form the matrix $X = A \cdot V \cdot \text{inv}(\text{diag}(L, I))$, followed by the QR factorization $X = UA \cdot LA$. Thus, $A = UA \cdot LA \cdot \text{diag}(L, I) \cdot V'$ and $B = L \cdot V'$. Then deflation and refinement (optional) are employed to produce a rank-revealing decomposition. The deflation procedure is based on the generalized LINPACK condition estimator, and the refinement steps on QR-iterations.

See Also

`ullv` – Rank-revealing ULLV algorithm, B full column rank.

References

- [1] F.T. Luk and S. Qiao, “A New Matrix Decomposition for Signal Processing”, *Automatica*, 30 (1994), pp. 39–43.
- [2] F.T. Luk and S. Qiao, “An adaptive algorithm for interference cancelling in array processing; in F.T. Luk (Ed.), “Advanced Signal Processing Algorithms, Architectures, and Implementations VI,” SPIE Proceedings, Vol. 2846 (1996), pp. 151-161.

ulliv_up_a

Purpose

Update the A-part of the rank-revealing ULLIV decomposition.

Synopsis

```
[p,LA,L,V,UA,UB,vec] = ulliv_up_A(p,LA,L,V,UA,UB,a)
[p,LA,L,V,UA,UB,vec] = ulliv_up_A(p,LA,L,V,UA,UB,a,tol_rank)
[p,LA,L,V,UA,UB,vec] = ulliv_up_A(p,LA,L,V,UA,UB,a,tol_rank,tol_ref,max_ref)
[p,LA,L,V,UA,UB,vec] = ulliv_up_A(p,LA,L,V,UA,UB,a,tol_rank,tol_ref,max_ref,fixed_rank)
```

Description

Given a rank-revealing ULLIV decomposition of the m_A -by- n matrix with $m_A \geq n$, and the full-rank m_B -by- n matrix $B = UB*L*V'$ with $m_B < n$, the function computes the updated decomposition

$$\begin{bmatrix} A \\ a \end{bmatrix} = UA*LA*\begin{bmatrix} L & 0 \\ 0 & I \end{bmatrix}*V' \quad \text{and} \quad B = UB*\begin{bmatrix} L & 0 \\ 0 & I \end{bmatrix}*V'$$

where a is the new row added to A . Note that B must have full row rank, that the row dimension of UA will increase by one, and that the matrices UA and UB can be left out by inserting an empty matrix $[]$ while V is required.

Input Parameters

| | |
|----------------------|--|
| p | numerical rank of $A*\text{pinv}(B)$ revealed in LA ; |
| LA,L,V,UA,UB | the ULLIV factors of A and B ; |
| a | the new row added to A ; |
| tol_rank | rank decision tolerance; |
| tol_ref | upper bound on the 2-norm of the off-diagonal block $LA(p+1:m_B,1:p)$ relative to the Frobenius-norm of LA ; |
| max_ref | max. number of refinement steps per singular value to achieve the upper bound tol_ref ; |
| fixed_rank | if true, deflate to the fixed rank given by p instead of using the rank decision tolerance; |
| Defaults | $\text{tol_rank} = \text{sqrt}(n)*\text{norm}(LA,1)*\text{eps}$; $\text{tol_ref} = 1e-04$; $\text{max_ref} = 0$; |

Output Parameters

`p` numerical rank of updated quotient;
`LA,L,V,UA,UB` the updated ULLV factors;

`vec` a 5-by-1 vector with:
`vec(1)` = upper bound of $\text{norm}(LA(p+1:mB,1:p))$,
`vec(2)` = estimate of p th singular value,
`vec(3)` = estimate of $(p+1)$ th singular value,
`vec(4)` = a posteriori upper bound of num. nullspace angle,
`vec(5)` = a posteriori upper bound of num. range angle.

See Also

`ulliv_up_B` – Update the B-part of the rank-revealing ULLIV decomp.

References

- [1] F.T.Luk and S. Qiao, “A New Matrix Decomposition for Signal Processing”, *Automatica*, 30 (1994), pp. 39–43.
- [2] F.T.Luk and S. Qiao, “An adaptive algorithm for interference cancelling in array processing; in F.T. Luk (Ed.), “Advanced Signal Processing Algorithms, Architectures, and Implementations VI,” SPIE Proceedings, Vol. 2846 (1996), pp. 151-161.

ulliv_up_B

Purpose

Update the B-part of the rank-revealing ULLIV decomposition.

Synopsis

```
[p,LA,L,V,UA,UB,vec] = ulliv_up_B(p,LA,L,V,UA,UB,b)
[p,LA,L,V,UA,UB,vec] = ulliv_up_B(p,LA,L,V,UA,UB,b,tol_rank)
[p,LA,L,V,UA,UB,vec] = ulliv_up_B(p,LA,L,V,UA,UB,b,tol_rank,tol_ref,max_ref)
[p,LA,L,V,UA,UB,vec] = ulliv_up_B(p,LA,L,V,UA,UB,b,tol_rank,tol_ref,max_ref,fixed_rank)
```

Description

Given a rank-revealing ULLIV decomposition of the m_A -by- n matrix with $m_A \geq n$, and the full-rank m_B -by- n matrix $B = UB*L*V'$ with $m_B < n$, the function computes the updated decomposition

$$A = UA*LA*\begin{bmatrix} L & 0 \\ 0 & I \end{bmatrix}*V' \quad \text{and} \quad \begin{bmatrix} B \\ b \end{bmatrix} = UB*\begin{bmatrix} L & 0 \\ 0 & I \end{bmatrix}*V'$$

where b is the new row added to B . Note that the updated matrix $[B;b]$ must have full row rank, that the row dimension of UB will increase by one, and that the matrices UA and UB can be left out by inserting an empty matrix $[]$ while V is required.

Input Parameters

| | |
|----------------|--|
| p | numerical rank of $A*\text{pinv}(B)$ revealed in LA ; |
| LA,L,V,UA,UB | the ULLIV factors of A and B ; |
| b | the new row added to B ; |
| tol_rank | rank decision tolerance; |
| tol_ref | upper bound on the 2-norm of the off-diagonal block $LA(p+1:m_B,1:p)$ relative to the Frobenius-norm of LA ; |
| max_ref | max. number of refinement steps per singular value to achieve the upper bound tol_ref ; |
| $fixed_rank$ | if true, deflate to the fixed rank given by p instead of using the rank decision tolerance; |
| Defaults | $tol_rank = \text{sqrt}(n)*\text{norm}(LA,1)*\text{eps}$; $tol_ref = 1e-04$; $max_ref = 0$; |

Output Parameters

`p` numerical rank of updated quotient;
`LA,L,V,UA,UB` the updated ULLV factors;

`vec` a 5-by-1 vector with:
`vec(1)` = upper bound of $\text{norm}(LA(p+1:mB,1:p))$,
`vec(2)` = estimate of p th singular value,
`vec(3)` = estimate of $(p+1)$ th singular value,
`vec(4)` = a posteriori upper bound of num. nullspace angle,
`vec(5)` = a posteriori upper bound of num. range angle.

See Also

`ulliv_up_A` – Update the A-part of the rank-revealing ULLIV decomp.

References

- [1] F.T.Luk and S. Qiao, “A New Matrix Decomposition for Signal Processing”, *Automatica*, 30 (1994), pp. 39–43.
- [2] F.T.Luk and S. Qiao, “An adaptive algorithm for interference cancelling in array processing; in F.T. Luk (Ed.), “Advanced Signal Processing Algorithms, Architectures, and Implementations VI,” SPIE Proceedings, Vol. 2846 (1996), pp. 151-161.

vsv_qrit

Purpose

Refinement of VSV decomposition via block QR-iterations.

Synopsis

```
[L] = vsv_qrit(p,num_ref,L)
[L,V] = vsv_qrit(p,num_ref,L,[],V)
[L,Omega] = vsv_qrit(p,num_ref,L,Omega)
[L,Omega,V] = vsv_qrit(p,num_ref,L,Omega,V)
[R,Omega] = vsv_qrit(p,num_ref,R,Omega)
[R,Omega,V] = vsv_qrit(p,num_ref,R,Omega,V)
```

Description

Given a VSV decomposition with numerical rank p , of one of the forms

$$\begin{aligned} A &= V*L'*L*V' && \text{(semidefinite } A, \text{ lower triangular } L) \\ A &= V*L'*\Omega*L*V' && \text{(indefinite } A, \text{ lower triangular } L) \\ A &= V*R'*\Omega*R*V' && \text{(indefinite } A, \text{ upper triangular } R) \end{aligned}$$

the function refines the rank-revealing decomposition via `num_ref` steps of block QR iterations applied to the triangular matrix.

Input Parameters

`p` numerical rank of A ;
`num_ref` number of refinement iterations;
`T` triangur matrix (L or R , depending on VSV decomposition);
`Omega` signature matrix (indef. case) or empty (semidef. case);
`V` orthogonal matrix;

Output Parameters

`T` refined triangular matrix
`Omega` or `V` refined Ω (indef. case) or refined V (semidef. case)
`V` refined V (indef. case)

Algorithm

Refinement is identical to block QR iteration, in which the off-diagonal block of the triangular matrix is “flipped” to the diagonally opposite position and then back again.

See Also

`ulv_ref` – Refine one column of L in the ULV decomposition.
`urv_ref` – Refine one column of R in the URV decomposition.

References

- [1] R. Mathias and G.W. Stewart, “A Block QR Algorithm and the Singular Value Decomposition”, *Lin. Alg. Appl.*, 182 (1993), pp. 91–100.

vsvd_L_mod

Purpose

Rank-one modification of VSV decomp. of sym. indef. matrix, L version.

Synopsis

```
[p,L,Omega,V] = vsvd_L_mod(p,L,Omega,V,omega,v)
[p,L,Omega,V] = vsvd_L_mod(p,L,Omega,V,omega,v,tol_rank)
[p,L,Omega,V] = vsvd_L_mod(p,L,Omega,V,omega,v,tol_rank,inv_iter)
[p,L,Omega,V] = vsvd_L_mod(p,L,Omega,V,omega,v,tol_rank,inv_iter,fixed_rank)
```

Description

Given a rank-revealing VSV decomposition of a symmetric indefinite matrix $A = V*(L'*Omega*L)*V'$, the function computes the updated rank-revealing decomposition of the matrix $A + omega*v*v'$, where $omega = +1$ or -1 .

Input Parameters

| | |
|------------|---|
| p | numerical rank of A; |
| L | lower triangular matrix in $A = V*(L'*Omega*L)*V'$; |
| Omega | signature matrix in $A = V*(L'*Omega*L)*V'$; |
| V | orthogonal matrix in $A = V*(L'*Omega*L)*V'$; |
| omega | update (+1) or downdate (-1); |
| v | rank-one update column vector; |
| tol_rank | rank decision tolerance; |
| inv_iter | number of inverse iterations per deflation step; |
| fixed_rank | deflate to the fixed rank given by fixed_rank instead of using the rank decision tolerance; |
| Defaults | tol_rank = $n*\text{norm}(L,1)*\text{eps}$; inv_iter = 5; |

Output Parameters

| | |
|-------|------------------------------------|
| p | numerical rank of modified matrix; |
| L | updated lower triangular matrix; |
| Omega | updated signature matrix; |
| V | updated orthogonal matrix; |

See Also

vsvd_R_mod – Rank-one mod. of VSV decomp. of sym. indef. matrix, R version.
vsvd_up – Rank-one update of VSV decomposition of semidefinite matrix.

References

- [1] P.C. Hansen & P.Y. Yalamov, "Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization", *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.

vsvid_R_mod

Purpose

Rank-one modification of VSV decomp. of indef. matrix, R version.

Synopsis

```
[p,R,Omega,V] = vsvid_R_mod(p,R,Omega,V,omega,v)
[p,R,Omega,V] = vsvid_R_mod(p,R,Omega,V,omega,v,tol_rank)
[p,R,Omega,V] = vsvid_R_mod(p,R,Omega,V,omega,v,tol_rank,inv_iter)
[p,R,Omega,V] = vsvid_R_mod(p,R,Omega,V,omega,v,tol_rank,inv_iter,fixed_rank)
```

Description

Given a rank-revealing VSV decomposition of a symmetric indefinite matrix $A = V*(R'*Omega*R)*V'$, the function computes the updated rank-revealing decomposition of the matrix $A + omega*v*v'$, where $omega = +1$ or -1 .

Input Parameters

| | |
|------------|---|
| p | numerical rank of A; |
| R | upper triangular matrix in $A = V*(R'*Omega*R)*V'$; |
| Omega | signature matrix in $A = V*(R'*Omega*R)*V'$; |
| V | orthogonal matrix in $A = V*(R'*Omega*R)*V'$; |
| omega | update (+1) or downdate (-1); |
| v | rank-one update column vector; |
| tol_rank | rank decision tolerance; |
| inv_iter | number of inverse iterations per deflation step; |
| fixed_rank | deflate to the fixed rank given by fixed_rank instead of using the rank decision tolerance; |
| Defaults | tol_rank = $n*\text{norm}(R,1)*\text{eps}$; inv_iter = 5; |

Output Parameters

| | |
|-------|------------------------------|
| p | numerical rank of updated A; |
| R | updated upper triangular; |
| Omega | updated signature matrix; |
| V | updated orthogonal matrix; |

See Also

vsvid_mod – Rank-one modification of VSV decomposition of indefinite matrix.
vsvsd_up – Rank-one update of VSV decomposition of semidefinite matrix.

References

- [1] P.C. Hansen & P.Y. Yalamov, “Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization”, *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.

vsvd_ip

Purpose

Interim process for indefinite VSV algorithm.

Synopsis

$[W,C,\Omega] = \text{vsvd_ip}(L,D)$

Input Parameters

L,D Factors in LDL^T factorization;

Output Parameters

W,C,Ω Matrices in $L*D*L' = W*C'*\Omega*C*W'$.

Algorithm

The factorization $L*D*L'$ is replaced with $W*C'*\Omega*C*W'$, where W is orthogonal, C is upper triangular, and Ω is a signature matrix. This is accomplished via small eigenvalue decompositions of the 1-by-1 and 2-by-2 blocks of D .

References

- [1] P.C. Hansen, & P.Y. Yalamov, "Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization", *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.

vsvsd_up

Purpose

Rank-one update of VSV decomposition of semidefinite matrix.

Synopsis

```
[p,L,V] = vsvsd_up(p,L,V,v)
[p,L,V] = vsvsd_up(p,L,V,v,tol_rank)
[p,L,V] = vsvsd_up(p,R,V,v,tol_rank,fixed_rank)
```

Description

Given a rank-revealing VSV decomposition of a symmetric semidefinite matrix $A = V*(L'*L)*V'$, the function computes the updated rank-revealing decomposition of $A + v*v'$. Use function `vsvsd_mod` with `omega = -1` to downdate the VSV decomposition of a symmetric semidefinite matrix.

Input Parameters

| | |
|-------------------------|--|
| <code>p</code> | numerical rank of A ; |
| <code>L</code> | lower triangular matrix in $A = V*(L'*L)*V'$; |
| <code>V</code> | orthogonal matrix in $A = V*(L'*L)*V'$; |
| <code>v</code> | rank-one update column vector; |
| <code>tol_rank</code> | rank decision tolerance; |
| <code>fixed_rank</code> | deflate to the fixed rank given by <code>fixed_rank</code> instead of using the rank decision tolerance; |
| Defaults | <code>tol_rank = n*norm(L,1)*eps</code> ; |

Output Parameters

| | |
|----------------|----------------------------------|
| <code>p</code> | numerical rank of updated A ; |
| <code>L</code> | updated lower triangular matrix; |
| <code>V</code> | updated orthogonal matrix; |

See Also

`vsvsd_L_mod` – Rank-one mod. of VSV decomp. of sy., indef. matrix, L version.
`vsvsd_R_mod` – Rank-one mod. of VSV decomp. of sy., indef. matrix, R version.

References

- [1] P.C. Hansen & P.Y. Yalamov, “Computing Symmetric Rank-Revealing Decompositions via Triangular Factorization”, *SIAM J. Matrix Anal. Appl.*, 23 (2001), pp. 443–458.