# Towards a Fast and Robust $\mathcal{O}(n^2)$ Algorithm for the Bidiagonal SVD

Paul R. Willems

Applied Computer Science and Scientific Computing, University of Wuppertal, D-42097 Wuppertal, Germany, willems@math.uni-wuppertal.de

**Abstract.** We describe a new algorithm for computing the singular value decomposition of a real bidiagonal matrix, which uses ideas developed by Großer and Lang that extend the MRRR algorithm by Dhillon and Parlett for the tridiagonal symmetric eigenproblem. This new algorithm inherits all the favorable properties of the MRRR algorithm, like speed, accuracy, easy parallelization and especially adaptivity (i.e. for a bidiagonal matrix of dimension $n$, $k \leq n$ singular triplets can be computed with $\mathcal{O}(kn)$ operations). It is planned that this algorithm will be included in the next release of the LAPACK library.

## Background and Outline of this presentation

For computing the singular value decomposition (bSVD) of a real square bidiagonal matrix $B \in \mathbb{R}^n$ the standard approach is to reduce the problem to the symmetric tridiagonal eigenproblem (tSEP). To this end, one can use the so-called *normal equations* $B^T B$ and $BB^T$ or the Golub-Kahan-Matrix $T_{\text{GK}}$, which is a symmetric tridiagonal matrix resulting from permuting the Jordan-Wielandt-Form of $B$:

$$T_{\text{GK}} = P^T \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} P.$$

For tSEP, a valuable theoretical improvement has been made by the quite recent discovery of the algorithm of Multiple Relatively Robust Representations (MRRR, or MR$^3$) by Dhillon and Parlett [1–5]. In short this algorithm can be described as a variant of inverse iteration [6]. For eigenvalues whose *relative* distance to the rest of the spectrum is large enough so-called *twisted factorizations* are used to compute the corresponding eigenvector accurately. For each of the remaining *clusters* of eigenvalues the algorithms chooses a shift close to the cluster and proceeds recursively for the eigenpairs within the cluster (note that absolute distances between eigenvalues are shift-invariant, whereas relative distances are not). Thus the computational flow can be described as traversing a special tree-like structure, the *representation tree.* Two additional ingredients of the algorithm guarantee that the eigenvectors which are computed from a (successively) shifted version of the original matrix are indeed worth the effort and not spoiled by the shifting process. Firstly, to compute the shifted matrices, highly accurate algorithms based on the dqds transformation [7, 8] are employed, which are mixed relatively stable. And secondly, the algorithm makes sure that the matrices encountered in the tree define the eigenpairs of interest to high relative accuracy, i.e., that they are *Relatively Robust Representations*.

In order to enjoy the benefits of the MRRR algorithm also when solving the bSVD, Großer discovered in his thesis [9] that due to numerical problems it is not sufficient to apply MRRR to the Golub-Kahan-Matrix or the normal equations $B^TB$ and $BB^T$ in a black box fashion. In essence, the shifting process inherent in MRRR destroys in both cases necessary information for the singular value decomposition of the matrix $B$. To overcome these problems, Großer and Lang proposed so called *coupling relations* [10, 11] which allow to run MRRR implicitly on all three matrices in parallel, but without spoiling the SVD of $B$.

In an ongoing research project we are working on the refinement and extension of this approach. The task to fuse the MRRR algorithm with the couplings into an efficient and robust implementation alone is not trivial, but so far the result can be favorably compared to the Divide & Conquer algorithm [12]. Further research focuses on optimization, theoretical foundation and simplification of the method and the incorporation of additional techniques like the submatrix method by Parlett [13]. It is planned that the algorithm will be incorporated into the next release of the LAPACK [14] library.

The first part of this talk will give a gentle overview of the MRRR algorithm and the coupling approach for the bSVD. The second part will delve deeper into theoretical background and techniques for practical realisation of the algorithm. Finally, we will present up to date results of numerical tests comparing our implementation to the QR and Divide & Conquer implementations from LAPACK.

## Acknowledgements

This presentation covers joint work with Bruno Lang. We are indebted to James Demmel, Osni Marques, Beresford Parlett and Christof Vömel for keeping us up-to-date on the constant improvements in the MRRR algorithm, its implementation and its testing environment.

## References

1. Dhillon, I.S.: A new $O(n^2)$ algorithm for the symmetric tridiagonal eigenvalue/eigenvector problem. PhD thesis, University of California, Berkeley (1997)
2. Parlett, B.N., Dhillon, I.S.: Fernando's solution to Wilkinson's problem: an application of double factorization. Linear Algebra and its Applications **267** (1997) 247–279
3. Dhillon, I.S., Parlett, B.N.: Multiple representations to compute orthogonal eigenvectors of symmetric tridiagonal matrices. Linear Algebra and its Applications **387** (2004) 1–28
4. Dhillon, I.S., Parlett, B.N.: Orthogonal eigenvectors and relative gaps. SIAM Journal on Matrix Analysis and Applications **25**(3) (2004) 858–899

5. Parlett, B.N., Dhillon, I.S.: Relatively robust representations of symmetric tridiagonals. Linear Algebra and its Applications **309** (2000) 121–151
6. Ipsen, I.C.F.: Computing an eigenvector with inverse iteration. SIAM Review **39**(2) (1997) 254–291
7. Fernando, K., Parlett, B.N.: Accurate singular values and differential qd algorithms. Numerische Mathematik **67** (1994) 191–229
8. Parlett, B.N., Marques, O.A.: An implementation of the dqds algorithm (positive case). Linear Algebra and its Applications **309** (2000) 217–259
9. Großer, B.: Ein paralleler und hochgenauer $O(n^2)$ Algorithmus für die bidiagonale Singulärwertzerlegung. PhD thesis, Bergische Universität Wuppertal, Fachbereich Mathematik, Wuppertal, Germany (2001) In German.
10. Großer, B., Lang, B.: An $O(n^2)$ algorithm for the bidiagonal SVD. Linear Algebra and its Applications **358** (2003) 45–70
11. Großer, B., Lang, B.: On symmetric eigenproblems induced by the bidiagonal SVD. SIAM Journal on Matrix Analysis and Applications **26**(3) (2005) 599–620
12. Willems, P.R., Lang, B., Vömel, C.: Computing the bidiagonal SVD using multiple relatively robust representations. To appear in SIAM Journal on Matrix Analysis and Applications. (Also as LAPACK Working Note #166.) (2005)
13. Parlett, B.N.: Invariant subspaces for tightly clustered eigenvalues of tridiagonals. BIT Num. Math. **36**(3) (1996) 542–562
14. Anderson, E., Bai, Z., Bischof, C., Blackford, S., Demmel, J., Dongarra, J., Croz, J.D., Greenbaum, A., Hammarling, S., McKenney, A., Sorensen, D.: LAPACK User's Guide. 3rd edn. SIAM, Philadelphia, PA (1999)