Cholesky-factor based implementation for doubling algorithms with permuted Lagrangian graph bases

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For a Hermitian matrix $X \in \mathbb{C}^{n\times n}$ and chosen indices $\mathcal{I} = (i_1, i_2, \ldots, i_k)$, where all i_j are distinct elements of $\{1, 2, \ldots, n\}$, a (symmetric) principal pivot transform (PPT) is the map $X \mapsto X'$, with X' given by

$$\begin{aligned} (X')_{\mathcal{I}\mathcal{I}} &= -X_{\mathcal{I}\mathcal{I}}^{-1}, & (X')_{\mathcal{I}\mathcal{I}^c} &= X_{\mathcal{I}\mathcal{I}}^{-1} X_{\mathcal{I}\mathcal{I}^c}, \\ (X')_{\mathcal{I}^c\mathcal{I}} &= X_{\mathcal{I}^c\mathcal{I}} X_{\mathcal{I}\mathcal{I}}^{-1}, & (X')_{\mathcal{I}^c\mathcal{I}^c} &= X_{\mathcal{I}^c\mathcal{I}^c} - X_{\mathcal{I}^c\mathcal{I}} X_{\mathcal{I}\mathcal{I}}^{-1} X_{\mathcal{I}\mathcal{I}^c}. \end{aligned}$$

In the above formulae, $\mathcal{I}^c$ contains all indices that are not in $\mathcal{I}$ and $X_{\mathcal{I}\mathcal{J}}$ is a submatrix of X whose rows and columns are indexed by $\mathcal{I}$ and $\mathcal{J}$, respectively. This map is used by Mehrmann and Poloni in [2] to solve algebraic Riccati equations and represent certain families of structured matrix pencils by computing matrices whose elements are bounded by a small constant, which helps numerical stability.

Most of the matrices X needed in the algorithms from [2] have definiteness properties (which are crucial, for instance, in proving their convergence): they belong to the class of quasidefinite matrices, i.e., they are 2×2 Hermitian block matrices with a negative definite leading and a positive definite trailing diagonal block. However, in [2] definiteness is not used or enforced in the PPTs.

In this work we present a theory describing the structure preserving transformations of the definite blocks and develop an algorithm to implement PPTs in factored form that keeps these definiteness properties exactly. Specifically, we represent a quasidefinite X in a factored-diagonal block form via a triple of matrices (A, B, C) and show how to efficiently implement the PPT

$$X := \begin{bmatrix} -A^*A & B^* \\ B & CC^* \end{bmatrix} \mapsto \begin{bmatrix} -(A')^*A' & B'^* \\ B' & C'C'^* \end{bmatrix} =: X'$$

directly on the triple. Similarly to [2], the index set of interest for the PPT is either $\mathcal{I} = \{i\}$ or $\mathcal{I} = \{i, j\}$. The former corresponds to the leading block of X either shrinking or growing in size by 1 and we show that the latter case only involves i and j that correspond to the indices defining B.

The cost of using the factored form is a more involved way of determining a single pivot, $\mathcal{I} = \{i\}$: while in [2] this is done by simply finding a diagonal element of X above a certain threshold, here it involves the column norms of A and the row norms of C. We are faced with the same problem of updating or recomputing the norms as in the rank-revealing QR and therefore use the heuristic from [1] to switch between the two.

As a final contribution, we show that using the factors in PPTs allows us to improve the bound on certain elements in the final solution for this type of problems.

References

[1] Z. Drmač and Z. Bujanović. On the failure of rank-revealing QR factorization software – a case study. *ACM Trans. Math. Software*, 35(2):12:1–12:28, July 2008.

[2] V. Mehrmann and F. Poloni. Doubling algorithms with permuted Lagrangian graph bases. *SIAM J. Matrix Anal. Appl.*, 33(3):780–805, 2012.