Note on Trace Maximization Correction to the Multi-precision Polar Decomposition

Thomas Seleiro*

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1 Polar Decomposition

For $A \in \mathbb{C}^{m\times n}$, we can find a polar decomposition $A = UH$, where $U \in \mathbb{C}^{m\times n}$ has unitary columns and $H \in \mathbb{C}^{n\times n}$ is Hermitian positive semi-definite. The unitary polar factor U for an $n \times n$ matrix A can be computed via the scaled Newton iteration defined by the recursive step

$$X_{k+1} = \frac{1}{2}(\mu_k X_k + \mu_k^{-1} X_k^{-*}), \qquad X_0 = A.$$

Throughout the experiments performed, we used the $1, \infty$-norm scaling factor

$$\mu_k = \left(\frac{\|X_k^{-1}\|_1 \|X_k^{-1}\|_\infty}{\|X_k\|_1 \|X_k\|_\infty} \right)^{1/4},$$

and we use a mixture of the stopping conditions $\|X_k - X_{k-1}\|_\infty / \|X_k\|_\infty \leq nu$ and $\|I - X_k^* X_k\|_\infty \leq nu$ suggested in [1, §8.4].

We try to evaluate the effectiveness of using this method for computing the polar decomposition of a matrix in multiple precision. The iterates converge quadratically to the unitary polar factor. Therefore once the iteration has converged to a lower precision, only one further iteration in the desired higher precision would be needed for convergence.

The computed matrix U_1 will be unitary to the desired precision, but the corresponding Hermitian factor $H_1 = U_1^* A$ need not be Hermitian positive semi-definite. Table **??**. shows that H_1 is only Hermitian to single precision and the calculated matrices are inaccurate. We try to compensate for this inaccuracy

*Department of Mathematics, University of Manchester, Manchester, M13 9PL, UK (thomas.seleiro@postgrad.manchester.ac.uk)

Table 1

	t_G	t_N	s_G	$\|H_G - H_G^*\|/2$	$\|H_N - H_N^*\|/2$
`rand(25)`	0.27	1.67e-3	245	1.91e-14	8.12e-15
`rand(50)`	4.88	1.83e-3	713	7.88e-14	3.90e-14
`rand(75)`	35.96	3.11e-3	1364	1.64e-13	9.17e-14
`rand(100)`	140.53	4.49e-3	2110	3.14e-13	1.46e-13

Table 2: Table showing t_G and t_N, the calculation times using `maxtracePoldec` and a double precision Newton iteration; s_G the number of sweeps of `maxtracePoldec`, and the norm skew-Hermitian parts of the calculated Hermitian polar factors.

by calculating the polar decomposition $H_1 = WH$. We then have $A = U_1 H_1 = (U_1 W)H =: UH$, where U is unitary to double precision and H is Hermitian positive semi-definite.

In general, H_1 is not unitary ($\|A\|_2 = \|U_1 H_1\|_2 = \|H_1\|_2$). Therefore we cannot use the Newton method to compute this polar decomposition, since the iterates converge to a unitary matrix.

We instead use the property that for all unitary $W \in \mathbb{C}^{n\times n}$, trace$(W^*A)$ is maximised if and only if W is a unitary polar factor of A (see [1, Prob. 8.13]).

An algorithm for computing the polar decomposition is proposed in [2, p.84]. We repeatedly loop through every 2×2 submatrix $A_{ij} = A([i,j],[i,j])$ and apply Givens transformations that make A_{ij} symmetric and maximise its trace. We do so until the matrix is symmetric. If the resulting matrix $\tilde{A}$ is indefinite, we apply a Householder transformation W^* where $W = I - 2xx^*$ where x is the normalized eigenvector of the smallest eigenvalue of $\tilde{A}$. This makes the resulting matrix symmetric positive semi-definite and increases the trace of $\tilde{A}$.

References

[1] N. J. Higham, *Functions of Matrices : Theory and Computation*, Society for Industrial and Applied Mathematics, Philadelphia, Pa, 2008.

[2] M. I. Smith, *Numerical Computation of Matrix Function*, PhD thesis, University of Manchester, Manchester, England, 2002.