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COMPUTING THE POLAR DECOMPOSITION—WITH APPLICATIONS*

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Abstract. A quadratically convergent Newton method for computing the polar decomposition of a full-rank matrix is presented and analysed. Acceleration parameters are introduced so as to enhance the initial rate of convergence and it is shown how reliable estimates of the optimal parameters may be computed in practice.

To add to the known best approximation property of the unitary polar factor, the Hermitian polar factor H of a nonsingular Hermitian matrix A is shown to be a good positive definite approximation to A and $\frac{1}{2}(A+H)$ is shown to be a best Hermitian positive semi-definite approximation to A. Perturbation bounds for the polar factors are derived.

Applications of the polar decomposition to factor analysis, aerospace computations and optimisation are outlined; and a new method is derived for computing the square root of a symmetric positive definite matrix.

Key words. polar decomposition, singular value decomposition, Newton's method, matrix square root

AMS(MOS) subject classifications. 65F25, 65F30, 65F35

1. Introduction.

The polar decomposition is a generalisation to matrices of the familiar complex number representation $z = re^{i\theta}$, $r \geqq 0$.

THEOREM 1.1. *Polar Decomposition. Let $A \in \mathbb{C}^{m\times n}$, $m \geqq n$. Then there exists a matrix $U \in \mathbb{C}^{m\times n}$ and a unique Hermitian positive semi-definite matrix $H \in \mathbb{C}^{n\times n}$ such that*

$$A = UH, \qquad U^*U = I_n.$$

If rank $(A) = n$ *then H is positive definite and U is uniquely determined.*

The decomposition is well known and can be found in many textbooks, for example, [13], [16], [27]. An early reference is [1].

It is well known that the polar factor U possesses a best approximation property (see § 2.2). Less attention has been paid in the literature to the Hermitian polar factor H. We derive some interesting properties of H which show that when A is nonsingular and Hermitian, H is a good Hermitian positive definite approximation to A and $\frac{1}{2}(A+H)$ is a best Hermitian positive semi-definite approximation to A.

In view of the properties possessed by the polar factors of a matrix, techniques for computing the polar decomposition are of interest. While U and H can be obtained via the singular value decomposition (see § 3.1), this approach is not always the most efficient (if $A \approx U$, as explained in § 6.2) or the most convenient (a library routine for computing the singular value decomposition might not be available, on a microcomputer, for example).

In § 3 we present and analyse a Newton method for computing the polar decomposition which involves only matrix additions and matrix inversions. The method is shown to be quadratically convergent. Acceleration parameters are introduced so as to enhance the initial rate of convergence and it is shown how reliable estimates of the optimal parameters may be computed in practice. The stability of the method is considered in § 4. In § 5 the relationship of the method to two well-known iterations is described.

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In § 6 we describe applications of the polar decomposition to factor analysis, aerospace computations and optimisation. We show how our algorithm may be employed in these applications and compare it with other methods in use currently. A new method for computing the square root of a symmetric positive definite matrix is derived.

2. Properties of the polar decomposition.

2.1. Elementary properties. We begin by noting the close relationship of the polar decomposition to the singular value decomposition. Let $A \in \mathbb{C}^{m\times n}$, $m \geqq n$, have the singular value decomposition [16, p. 16]

$$A = P\begin{pmatrix}\Sigma\\ 0\end{pmatrix}Q^*, \tag{2.1}$$

where $P \in \mathbb{C}^{m\times m}$ and $Q \in \mathbb{C}^{n\times n}$ are unitary and

$$\Sigma = \operatorname{diag}(\sigma_1, \sigma_2, \cdots, \sigma_n), \qquad \sigma_1 \geqq \sigma_2 \geqq \cdots \geqq \sigma_n \geqq 0.$$

Partitioning

$$P = [\underset{n}{P_1}, \underset{m-n}{P_2}], \qquad P_1^*P_1 = I_n,$$

it follows that A has the polar decomposition $A = UH$, where

$$U = P_1Q^*, \tag{2.2}$$

$$H = Q\Sigma Q^*. \tag{2.3}$$

Conversely, given the polar decomposition $A = UH \in \mathbb{C}^{n\times n}$, from a spectral decomposition $H = Q\Sigma Q^*$ ($Q^*Q = I$) one can construct the singular value decomposition $A = (UQ)\Sigma Q^*$.

Several interesting properties of the polar decomposition are displayed in Lemma 2.1. Our notation is as follows. For $A \in \mathbb{C}^{n\times n}\lambda(A)$ and $\sigma(A)$ denote, respectively, the set of eigenvalues and the set of singular values of A, and $\kappa_2(A) = \sigma_1/\sigma_n$ is the 2-norm condition number. $C^{1/2}$ denotes the unique Hermitian positive semi-definite square root of the Hermitian positive semi-definite matrix C [20], [27]. A is normal if $A^*A = AA^*$ [16, p. 193].

LEMMA 2.1. *Let $A \in \mathbb{C}^{n\times n}$ have the polar decomposition $A = UH$. Then*

(i) $H = (A^*A)^{1/2}$.

(ii) $\lambda(H) = \sigma(H) = \sigma(A)$.

(iii) $\kappa_2(H) = \kappa_2(A)$.

(iv) *A is normal if and only if $UH = HU$.*

Proof. (i)-(iii) are immediate. For (iv) see [13, p. 276].

2.2. The unitary polar factor. Our interest in the polar decomposition stems from a best approximation property possessed by the unitary factor. The following result displays this property; it is the generalisation to complex matrices of a result in [16, p. 425] (see also [9], [15], [17], [26], [31]). The Frobenius matrix norm is defined by

$$\|A\|_F = (\operatorname{trace}(A^*A))^{1/2}.$$

THEOREM 2.2. *Let $A, B \in \mathbb{C}^{m\times n}$ and let $B^*A \in \mathbb{C}^{n\times n}$ have the polar decomposition*

$$B^*A = UH.$$

Then for any unitary $Z \in \mathbb{C}^{n\times n}$,

$$\|A - BU\|_F \leqq \|A - BZ\|_F \leqq \|A + BU\|_F. \tag{2.4}$$

$$\|A \pm BU\|_F^2 = \sum_{i=1}^{n} (\sigma_i(A)^2 \pm 2\sigma_i(B^*A) + \sigma_i(B)^2). \tag{2.5}$$

An important special case of Theorem 2.2 is obtained by taking $m = n$ and $B = I$.

COROLLARY 2.3. *Let $A \in \mathbb{C}^{n\times n}$ have the polar decomposition*

$$A = UH.$$

Then for any unitary $Z \in \mathbb{C}^{n\times n}$,

$$\left(\sum_{i=1}^{n} (\sigma_i(A)-1)^2\right)^{1/2} = \|A-U\|_F \leqq \|A-Z\|_F \leqq \|A+U\|_F = \left(\sum_{i=1}^{n} (\sigma_i(A)+1)^2\right)^{1/2}.$$

Thus if distance is measured in the Frobenius norm, the nearest unitary matrix to $A \in \mathbb{C}^{n\times n}$ is the unitary factor in the polar decomposition of A; and the furthest unitary matrix from A is minus this unitary factor. This result was established by Fan and Hoffman [12] for any unitarily invariant norm (thus it is valid for the 2-norm). It is not hard to show that Corollary 2.3 remains true when $A \in \mathbb{C}^{m\times n}$ with $m > n$ (this does not follow immediately from Theorem 2.2).

2.3. The Hermitian polar factor. As well as yielding a closest unitary matrix, the polar decomposition provides information about nearby Hermitian positive (semi-) definite matrices.

Let $A \in \mathbb{C}^{n\times n}$ be Hermitian with at least one negative eigenvalue and consider the problem of finding a small-normed perturbation $E = E^*$ such that $A+E$ is positive semi-definite. Define, for any Hermitian B,

$$\delta(B) = \min\{\|E\|_2 : B+E \text{ is Hermitian positive semi-definite}\}. \tag{2.6}$$

From the Courant–Fischer minimax theory [16, p. 269], any admissible E in the definition of $\delta(A)$ must satisfy

$$0 \leqq \lambda_n(A+E) \leqq \lambda_n(A) + \lambda_1(E),$$

where $\lambda_n(\cdot) \leqq \cdots \leqq \lambda_1(\cdot)$. Thus

$$\|E\|_2 \geqq |\lambda_1(E)| \geqq \lambda_1(E) \geqq -\lambda_n(A). \tag{2.7}$$

We now find a perturbation E for which this lower bound is attained. Let A have the spectral decomposition

$$A = Z\Lambda Z^* = \sum_{i=1}^{n} \lambda_i z_i z_i^*, \qquad Z^*Z = I. \tag{2.8}$$

For

$$E_p = -\sum_{i:\,\lambda_i<0} \lambda_i z_i z_i^*$$

(or $E = -\lambda_n I$) it is easily seen that $A+E_p$ is singular and Hermitian positive semi-definite, with $\|E_p\|_2 = -\lambda_n$. It follows from (2.6) and (2.7) that

$$\delta(A) = -\lambda_n(A) \quad (\lambda_n(A) < 0). \tag{2.9}$$

Now observe, from (2.8), that A has the polar decomposition $A = UH$, where

$$U = Z \operatorname{diag}(\operatorname{sign}(\lambda_i))Z^*, \qquad H = Z \operatorname{diag}(|\lambda_i|)Z^*. \tag{2.10}$$

It follows that

$$E_p = \tfrac{1}{2}(H - A). \tag{2.11}$$

Thus $\frac{1}{2}(A+H) = A + E_p$ is a nearest Hermitian positive semi-definite matrix to A in the 2-norm. This is a special case of a result obtained by Halmos [18] that applies to general non-Hermitian linear operators A.

We summarise our findings in the following lemma.

LEMMA 2.4. *Let $A \in \mathbb{C}^{n\times n}$ be Hermitian, with the polar decomposition $A = UH$. Then*

(i) $\delta(A) = \max\{0, -\lambda_n(A)\} = \frac{1}{2}\|A - H\|_2$.

(ii) $\frac{1}{2}(A+H)$ *is a best Hermitian positive semi-definite approximation to A in the 2-norm.*

(iii) *For any Hermitian positive (semi-) definite $X \in \mathbb{C}^{n\times n}$,*

$$\|A - H\|_2 \leq 2\|A - X\|_2.$$

(iv) *H and A have a common set of eigenvectors.*

The lemma shows that from the polar decomposition of a Hermitian matrix A we can obtain not only a best Hermitian positive semi-definite approximation to A, $\frac{1}{2}(A+H)$, but also, if A is nonsingular, a good Hermitian positive definite approximation to A, H itself. In § 6.3 we give an example of how the positive definite approximation may be utilised.

2.4. Perturbation bounds for the polar factors. It is of interest both for theoretical and for practical purposes (see § 4) to determine bounds for the changes induced in the polar factors of a matrix by perturbations in the matrix. The following theorem provides such bounds.

THEOREM 2.5. *Let $A \in \mathbb{C}^{n\times n}$ be nonsingular, with the polar decomposition $A = UH$. If $\varepsilon = \|\Delta A\|_F / \|A\|_F$ satisfies $\kappa_F(A)\varepsilon < 1$ then $A + \Delta A$ has the polar decomposition*

$$A + \Delta A = (U + \Delta U)(H + \Delta H),$$

where

$$\frac{\|\Delta H\|_F}{\|H\|_F} \leq \sqrt{2}\,\varepsilon + O(\varepsilon^2),$$

$$\frac{\|\Delta U\|_F}{\|U\|_F} \leq (1+\sqrt{2})\kappa_F(A)\varepsilon + O(\varepsilon^2).$$

Proof. Let $E = (1/\varepsilon)\Delta A$. Then $A + tE$ is nonsingular for $0 \leq t \leq \varepsilon$. Thus $A + tE$ has the polar decomposition

$$A + tE = U(t)H(t), \qquad 0 \leq t \leq \varepsilon, \tag{2.12}$$

where $H(t)$ is positive definite. We prove the theorem under the assumption that $U(t)$ and $H(t)$ are twice continuously differentiable functions of t; a rather similar but longer proof which does not require this assumption may be found in [22].

From (2.12),

$$H(t)^2 = (A + tE)^*(A + tE),$$

which gives, on differentiating [16, p. 4] and setting $t = 0$,

$$H\dot{H}(0) + \dot{H}(0)H = A^*E + E^*A.$$

Since $A = UH$, this can be written as

$$H\dot{H}(0) + \dot{H}(0)H = HF + F^*H, \tag{2.13}$$

where

$$F = U^*E.$$

Let H have the spectral decomposition

$$H = Z\Lambda Z^*, \qquad Z^*Z = I.$$

Performing a similarity transformation on (2.13) using Z gives

$$\Lambda\tilde{H} + \tilde{H}\Lambda = \Lambda\tilde{F} + \tilde{F}^*\Lambda,$$

where

$$\tilde{H} = Z^*\dot{H}(0)Z = (\tilde{h}_{ij}), \qquad \tilde{F} = Z^*FZ = (\tilde{f}_{ij}).$$

This equation has the solution

$$\tilde{h}_{ij} = \frac{\lambda_i\tilde{f}_{ij} + \tilde{f}_{ji}^*\lambda_j}{\lambda_i + \lambda_j}, \qquad 1 \leqq i, j \leqq n.$$

Using the Cauchy-Schwarz inequality,

$$|\tilde{h}_{ij}|^2 \leqq \frac{\lambda_i^2 + \lambda_j^2}{(\lambda_i + \lambda_j)^2}(|\tilde{f}_{ij}|^2 + |\tilde{f}_{ji}|^2) \leqq |\tilde{f}_{ij}|^2 + |\tilde{f}_{ji}|^2,$$

from which it follows that

$$\|\tilde{H}\|_F \leqq \sqrt{2}\|\tilde{F}\|_F.$$

Thus

$$\|\dot{H}(0)\|_F = \|\tilde{H}\|_F \leqq \sqrt{2}\|\tilde{F}\|_F = \sqrt{2}\|F\|_F = \sqrt{2}\|E\|_F. \tag{2.14}$$

A Taylor expansion gives

$$H + \Delta H \equiv H(\varepsilon) = H(0) + \varepsilon\dot{H}(0) + O(\varepsilon^2) = H + \varepsilon\dot{H}(0) + O(\varepsilon^2),$$

so that

$$\|\Delta H\|_F \leqq \varepsilon\|\dot{H}(0)\|_F + O(\varepsilon^2) \leqq \sqrt{2}\,\varepsilon\|E\|_F + O(\varepsilon^2).$$

The required bound is obtained by dividing throughout by $\|H\|_F = \|A\|_F$ and using $\|E\|_F = \|A\|_F$.

Now write (2.12) in the form $U(t) = (A + tE)H(t)^{-1}$ and differentiate, to obtain

$$\dot{U}(t) = EH(t)^{-1} - (A + tE)H(t)^{-1}\dot{H}(t)H(t)^{-1}.$$

Setting $t = 0$ gives

$$\dot{U}(0) = EH^{-1} - AH^{-1}\dot{H}(0)H^{-1} = (E - U\dot{H}(0))H^{-1},$$

and so, using (2.14),

$$\|\dot{U}(0)\|_F \leqq (1+\sqrt{2})\|E\|_F\|H^{-1}\|_F = (1+\sqrt{2})\|E\|_F\|A^{-1}\|_F.$$

From the Taylor series for $U(t)$,

$$\begin{aligned}\|\Delta U\|_F = \|U(\varepsilon) - U(0)\|_F &\leqq \varepsilon\|\dot{U}(0)\|_F + O(\varepsilon^2)\\ &\leqq (1+\sqrt{2})\varepsilon\|E\|_F\|A^{-1}\|_F + O(\varepsilon^2)\\ &= (1+\sqrt{2})\varepsilon\kappa_F(A) + O(\varepsilon^2),\end{aligned}$$

which gives the required bound, since $\|\Delta U\|_F/\|U\|_F = \|\Delta U\|_F/\sqrt{n} \leqq \|\Delta U\|_F$. □

3. Computing the polar decomposition.

3.1. Using the singular value decomposition. Our constructive derivation of the polar decomposition in § 2 suggests the following computational procedure:

(1) compute the singular value decomposition (2.1), forming only the first n columns P_1 of P;

(2) form U and H according to (2.2) and (2.3).

This method requires (when A is real) approximately $7mn^2+11/3n^3$ flops to compute P_1, Σ and Q, if we use the Golub-Reinsch SVD algorithm [16, p. 175], plus mn^2 flops to form U and $n^3/2$ flops to form H (see [16, p. 32] for a discussion of the term "flop"). Since the SVD algorithm is numerically stable and is readily available in library routines such as LINPACK [11] this SVD approach has much to recommend it.

We now develop an alternative method for computing the polar decomposition which does not require the use of sophisticated library routines and which, in certain circumstances (see § 6.2), is computationally much less expensive than the SVD technique. The method applies to nonsingular square matrices. If $A \in \mathbb{C}^{m\times n}$ with $m > n$ and rank $(A) = n$ then we can first compute a QR factorisation [16, p. 146] $A = QR$ (where $Q \in \mathbb{C}^{m\times n}$ has orthonormal columns and R is upper triangular and nonsingular) and then apply the method to R. The polar decomposition of A is given in terms of that of R by

$$A = QR = Q(U_R H_R) = (QU_R)H_R \equiv UH.$$

3.2. A Newton method. Consider the iteration (the real matrix version of which is discussed in [3], [4], [5], [6], [28])

$$X_0 = A \in \mathbb{C}^{n\times n}, \qquad \text{nonsingular,} \tag{3.1a}$$

$$X_{k+1} = \tfrac{1}{2}(X_k + X_k^{-*}), \qquad k = 0, 1, 2, \cdots, \tag{3.1b}$$

where X_k^{-*} denotes $(X_k^{-1})^*$. We claim that the sequence $\{X_k\}$ converges quadratically to the unitary polar factor in A's polar decomposition. To prove this we make use of the singular value decomposition

$$\begin{aligned} A &= P\Sigma Q^* \qquad (P^*P = Q^*Q = I_n) \\ &\equiv UH, \end{aligned}$$

where

$$U = PQ^*, \qquad H = Q\Sigma Q^*. \tag{3.2}$$

Define

$$D_k = P^* X_k Q. \tag{3.3}$$

Then from (3.1) we obtain

$$D_0 = \Sigma, \tag{3.4a}$$

$$D_{k+1} = \tfrac{1}{2}(D_k + D_k^{-*}). \tag{3.4b}$$

Since $D_0 \in \mathbb{R}^{n\times n}$ is diagonal with positive diagonal elements it follows by induction that the sequence $\{D_k\}$ is defined and that

$$D_k = \operatorname{diag}(d_i^{(k)}) \in \mathbb{R}^{n\times n}, \qquad d_i^{(k)} > 0. \tag{3.5}$$

Accordingly, (3.4) represents n uncoupled scalar iterations

$$\begin{aligned} d_i^{(0)} &= \sigma_i, \\ d_i^{(k+1)} &= \frac{1}{2}\left(d_i^{(k)} + \frac{1}{d_i^{(k)}}\right), \end{aligned} \qquad 1 \leqq i \leqq n,$$

which we recognise as Newton iterations for the square root of 1 with starting values the singular values of A.

Simple manipulations yield the relations (cf. [19, p. 84], [21])

$$d_i^{(k+1)} - 1 = \frac{1}{2d_i^{(k)}}(d_i^{(k)} - 1)^2, \qquad 1 \leqq i \leqq n, \tag{3.6}$$

$$\frac{d_i^{(k+1)} - 1}{d_i^{(k+1)} + 1} = \left(\frac{d_i^{(k)} - 1}{d_i^{(k)} + 1}\right)^2 = \cdots = \left(\frac{\sigma_i - 1}{\sigma_i + 1}\right)^{2^{k+1}} \equiv \eta_i^{2^{k+1}}, \qquad 1 \leqq i \leqq n. \tag{3.7}$$

Since A is nonsingular $|\eta_i| < 1$ for each i. It follows that $d_i^{(k)} - 1$ as $k \to \infty$ for each i, that is, $D_k \to I$, or equivalently, from (3.3) and (3.2)

$$\lim_{k\to\infty} X_k = U.$$

To analyse the rate of convergence we write (3.6) in the form

$$D_{k+1} - I = \tfrac{1}{2}(D_k - I)D_k^{-1}(D_k - I)$$

and pre- and post-multiply by P and Q^*, respectively, to obtain, from (3.2) and (3.3)

$$X_{k+1} - U = \tfrac{1}{2}(X_k - U)X_k^{-1}(X_k - U).$$

Furthermore, using (3.2), (3.3) and (3.7),

$$\begin{aligned} \|(X_{k+1} + U)^{-1}(X_{k+1} - U)\|_2 &= \|Q(D_{k+1} + I)^{-1}P^*P(D_{k+1} - I)Q^*\|_2 \\ &= \|(D_{k+1} + I)^{-1}(D_{k+1} - I)\|_2 \\ &= \max_{1\leqq i\leqq n}\left(\frac{d_i^{(k)} - 1}{d_i^{(k)} + 1}\right)^2 = \max_{1\leqq i\leqq n} \eta_i^{2^{k+1}}. \end{aligned}$$

Note from (3.3) and (3.5) that $d_1^{(k)}, \cdots, d_n^{(k)}$ are the singular values of X_k. We have proved the following.

THEOREM 3.1. *Let $A \in \mathbb{C}^{n\times n}$ be nonsingular and consider iteration* (3.1). *Each iterate X_k is nonsingular,*

$$\lim_{k\to\infty} X_k = U$$

where U is the unitary factor in the polar decomposition of A, and

$$\|X_{k+1} - U\|_2 \leqq \begin{cases} \dfrac{1}{2}\|X_k^{-1}\|_2\|X_k - U\|_2^2, & (3.8) \\[2ex] \|X_{k+1} + U\|_2\left(\max\limits_{1\leqq i\leqq n}\left|\dfrac{\sigma_i(X_k) - 1}{\sigma_i(X_k) + 1}\right|\right)^2, & (3.9) \\[2ex] \|X_{k+1} + U\|_2\left(\max\limits_{1\leqq i\leqq n}\left|\dfrac{\sigma_i(A) - 1}{\sigma_i(A) + 1}\right|\right)^{2^{k+1}}. & (3.10) \end{cases}$$

3.3. Accelerating convergence. The quadratic convergence of iteration (3.1) ensures rapid convergence in the final stages of the iteration: (3.8) implies that the number of correct significant figures will approximately be doubled on each step. Initially, however, the speed of convergence can be inordinately slow, as can be seen by considering $A = \alpha I$, for large $|\alpha|$, in (3.1) and (3.10).

We are led to the idea of scaling the matrix A, or more generally, scaling the current iterate at the start of each step, with the aim of hastening the onset of the ultimate phase of rapid convergence.

Consider the scaling $X_k \to \gamma_k X_k$, $\gamma_k > 0$. From (3.1b) we have

$$X_{k+1} = X_{k+1}(\gamma_k) = \frac{1}{2}\left(\gamma_k X_k + \frac{1}{\gamma_k} X_k^{-*}\right)$$

(thus γ_k can be regarded as an acceleration parameter), and from (3.9)

$$\|X_{k+1}(\gamma_k) - U\|_2 \leq \|X_{k+1}(\gamma_k) + U\|_2 \theta_k(\gamma_k)^2, \tag{3.11}$$

where

$$\theta_k(\gamma_k) = \max_{1 \leq i \leq n} \left| \frac{\gamma_k \sigma_i(X_k) - 1}{\gamma_k \sigma_i(X_k) + 1} \right|.$$

A natural choice for γ_k is the value $\gamma_{\text{opt}}^{(k)}$ which minimises $\theta_k(\gamma)$. A straightforward argument shows that

$$\gamma_{\text{opt}}^{(k)} = (\sigma_1(X_k)\sigma_n(X_k))^{-1/2}, \tag{3.12}$$

$$\theta_k(\gamma_{\text{opt}}^{(k)}) = \frac{\kappa_2(X_k)^{1/2} - 1}{\kappa_2(X_k)^{1/2} + 1}. \tag{3.13}$$

One can show that for $X_{k+1} = X_{k+1}(\gamma_{\text{opt}}^{(k)})$,

$$\begin{aligned} \kappa_2(X_{k+1}) &\leq \frac{1}{2}\left(\kappa_2(X_k)^{1/2} + \frac{1}{\kappa_2(X_k)^{1/2}}\right) \\ &\leq \kappa_2(X_k)^{1/2}. \end{aligned} \tag{3.14}$$

If this acceleration technique is used at each stage of iteration (3.1) then from (3.11), (3.13) and (3.14) we have, by induction (cf. (3.10))

$$\|X_{k+1} - U\|_2 \leq \|X_{k+1} + U\|_2 \left(\frac{\kappa_2(A)^{1/2^{k+1}} - 1}{\kappa_2(A)^{1/2^{k+1}} + 1}\right)^2. \tag{3.15}$$

The effectiveness of the acceleration procedure is illustrated by the example $A = \text{diag}(1, 2^4, 3^4, \cdots, 25^4)$; with the convergence criterion $\|X_k - U\|_2 \leq 10^{-9}$ the unaccelerated iteration requires twenty-two iterations, while the accelerated version requires only seven.

3.4. The practical algorithm. It is not feasible to compute $\gamma_{\text{opt}}^{(k)}$ exactly at each stage, since this would require computation of the extremal singular values of X_k, but a good approximation to $\gamma_{\text{opt}}^{(k)}$ can be computed at negligible cost.

Taking $A = X_k$, X_k^{-1} in the inequalities [16, p. 15]

$$\sigma_1(A) = \|A\|_2 \leq \sqrt{\|A\|_1 \|A\|_\infty} \leq \sqrt{n}\|A\|_2,$$

and defining

$$\alpha_k = \sqrt{\|X_k\|_1 \|X_k\|_\infty}, \qquad \beta_k = \sqrt{\|X_k^{-1}\|_1 \|X_k^{-1}\|_\infty},$$

$$\gamma_{\text{est}}^{(k)} = \sqrt{\frac{\beta_k}{\alpha_k}},$$

we find, from (3.12), that

$$\frac{1}{n^{1/4}} \gamma_{\text{opt}}^{(k)} \leq \gamma_{\text{est}}^{(k)} \leq n^{1/4} \gamma_{\text{opt}}^{(k)}.$$

Making suitable modifications to the derivation of (3.15) one can show that if the acceleration parameter estimates $\gamma_{\text{est}}^{(k)}$ are used in the first k stages of iteration (3.1) then (cf. (3.15))

$$\|X_{k+1}-U\|_2 \leq \|X_{k+1}+U\|_2\left(\frac{\sqrt{n}\,k_2(A)^{1/2^{k+1}}-1}{\sqrt{n}\,k_2(A)^{1/2^{k+1}}+1}\right)^2. \tag{3.16}$$

This bound suggests that in the initial stages of iteration (3.1) the estimates $\gamma_{\text{est}}^{(k)}$ will be almost as effective as the exact values $\gamma_{\text{opt}}^{(k)}$.

We have found empirically that once the error $\|X_k-U\|_2$ is sufficiently small—less than 10^{-2}, say—it is advantageous to revert to the original, unaccelerated form of iteration (3.1) so as to secure the desirable quadratic convergence.

Incorporating the acceleration parameter estimates $\gamma_{\text{est}}^{(k)}$ into iteration (3.1) we have the following.

ALGORITHM POLAR. Given a nonsingular matrix $A \in \mathbb{C}^{n\times n}$ this algorithm computes the polar decomposition $A = UH$.

(1) $X_0 := A$; $k := -1$.

(2) Repeat

$k := k+1$

$Y_k := X_k^{-1}$

If "close to convergence" then

$\gamma_k := 1$

else

$\alpha_k := \sqrt{\|X_k\|_1 \|X_k\|_\infty}$; $\quad \beta_k := \sqrt{\|Y_k\|_1 \|Y_k\|_\infty}$

$\gamma_k := \sqrt{\beta_k/\alpha_k}$

$$X_{k+1} := \frac{1}{2}\left(\gamma_k X_k + \frac{1}{\gamma_k} Y_k^*\right)$$

Until converged.

(3) $U := X_{k+1}$

$H_1 := U^*A$

$H := \frac{1}{2}(H_1 + H_1^*)$ (to ensure that the computed H is Hermitian).

Cost: (for real A) $(s+1)n^3$ flops, where s iterations are required for convergence.

In step (3) of the algorithm we could implicitly force H to be Hermitian by computing only the upper triangular part of U^*A; the given technique is preferred for reasons discussed in § 4.

A suitable convergence test to apply in step (2) of Algorithm Polar is

$$\|X_{k+1}-X_k\|_1 \leq \delta_n \|X_k\|_1, \tag{3.17}$$

where δ_n, depending on n, is a small multiple of the machine unit roundoff u [16, p. 33].

4. Backward error analysis. Consider the SVD approach to computing the polar decomposition, described in § 3.1. Using the backward error analysis for the Golub-Reinsch SVD algorithm [16, p. 174] one can show that the computed polar factors of A, $\hat{U}$ and $\hat{H}$, satisfy

$$\begin{aligned}
&\hat{U} = V+\Delta U, && \|\Delta U\|_2 \leq \varepsilon,\\
&\hat{H} = K+\Delta H, && \hat{H}^* = \hat{H}, \quad \|\Delta H\|_2 \leq \varepsilon \|K\|_2,\\
&VK = A+\Delta A, && \|\Delta A\|_2 \leq \varepsilon \|A\|_2,
\end{aligned}$$

where V is unitary, K is Hermitian positive semi-definite (certainly positive definite

if $\kappa_2(A) < 1/\varepsilon$) and ε is a small multiple of the machine precision u. Thus $\hat{U}$ and $\hat{H}$ are relatively close to the true polar factors of a matrix "near" to A. This result is the best that can be expected of any method for computing the polar decomposition in finite precision arithmetic.

We have been unable to prove a corresponding stability result for Algorithm Polar. Instead we derive an a posteriori test for stability of the computed polar factors $\hat{U}$ and $\hat{H}$.

Under mild assumptions one can show that with the convergence test (3.17) $\hat{U}$ satisfies

$$\hat{U} = V + \Delta U, \quad V^*V = I, \quad \|\Delta U\|_2 \leq \delta_n + O(\delta_n^2).$$

Algorithm Polar computes

$$\hat{H}_1 = \hat{U}^*A, \qquad \hat{H} = \tfrac{1}{2}(\hat{H}_1 + \hat{H}_1^*),$$

where, for simplicity, we ignore the rounding errors incurred in the computation of $\hat{H}_1$ and $\hat{H}$ (these lead to extra terms of order $\varepsilon\|A\|_2$, which do not affect the conclusion below). Defining

$$G = \tfrac{1}{2}(\hat{H}_1 - \hat{H}_1^*)$$

we have

$$V\hat{H} = V(\hat{H}_1 - G) = V(V^* + \Delta U^*)A - VG = A + \Delta A,$$

where

$$\|\Delta A\|_2 \leq \delta_n\|A\|_2 + \|G\|_2 + O(\delta_n^2).$$

This result is comparable with the result for the SVD method if (changing to the one-norm)

(4.1a) $$\delta_n \approx \varepsilon,$$

(4.1b) $$\|G\|_1 \approx \delta_n\|A\|_1,$$

(4.1c) $$\hat{H} \text{ is positive definite.}$$

Thus, in particular, $\|G\|_1$ must be sufficiently small, that is, $\hat{H}_1$ must be sufficiently close to being Hermitian. These conditions are easily tested; one can test (4.1c) by attempting to compute a Choleski decomposition of $\hat{H}$. Note that evaluation of (4.1b) is computationally much less expensive than the alternative of comparing $\|A - \hat{U}\hat{H}\|_1$ with $\delta_n\|A\|_1$.

Once the above tests have been performed, the accuracy of the computed polar factors (that is, the forward error) can be estimated with the aid of Theorem 2.5. The condition numbers $\kappa_1(A)$, $\kappa_\infty(A)$ can be formed at no extra cost during the first step of Algorithm Polar.

5. Relation to matrix sign and square root iterations. In this section we show how iteration (3.1) is related to iterations for the matrix sign function and the matrix square root.

For a diagonalisable matrix $A = ZDZ^{-1}$, $D = \text{diag}(d_i)$, $\text{Re}\, d_i \neq 0$, the sign function is given by [10], [30]

$$\text{sign}(A) = Z\,\text{diag}(\text{sign}(\text{Re}\, d_i))Z^{-1}.$$

An iterative method for computing sign (A) is [10], [30]

(5.1) $$S_{k+1} = \tfrac{1}{2}(S_k + S_k^{-1}), \qquad S_0 = A.$$

This iteration is essentially Newton's method for a square root of I, with starting matrix A (see [21]). We observe that iteration (3.1) implicitly performs this "sign iteration" on the matrix Σ of singular values: see (3.4) and (3.5). In fact, iteration (3.1) may be derived by applying the sign iteration to the Hermitian matrix

$$W = \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix},$$

whose eigenvalues are plus and minus the singular values of A.

Our analysis of the convergence of iteration (3.1), and of the acceleration parameters $\{\gamma_k\}$, applies with suitable modifications to the sign iteration (5.1); cf. [23], [24], [25], [30].

Consider now the iteration

$$Y_{k+1} = \tfrac{1}{2}(Y_k + Y_k^{-1}B), \qquad Y_0 = B, \tag{5.2}$$

for a square root of $B \in \mathbb{C}^{n\times n}$. In [21] this iteration is shown to be numerically unstable in the sense that a small perturbation in the kth iterate can lead to perturbations in succeeding iterates which grow unboundedly.

It can be shown that the sequence $\{X_k\}$ from iteration (3.1) is related to the sequence $\{Y_k\}$ generated by (5.2) with $B = A^*A$ according to

$$X_k^* A \equiv Y_k.$$

Thus iteration (3.1) implicitly carries out iteration (5.2) on $B = A^*A$, without ever forming A^*A. The techniques of [21] can be used to show that iteration (3.1) does not suffer from the numerical instability which impairs iteration (5.2).

6. Applications.

6.1. Factor analysis [17], [31]. In psychometrics the "Orthogonal Procrustes" problem consists of finding an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ which most nearly transforms a given matrix $B \in \mathbb{R}^{m\times n}$ into a given matrix $A \in \mathbb{R}^{m\times n}$, according to the criterion that the sum of squares of the residual matrix $A - BQ$ is minimised [17], [31] (see also [9], [32]). Theorem 2.2 shows that a solution to this problem is $Q = U$ where $B^TA = UH$ is a polar decomposition. If A and B have full rank then B^TA is nonsingular and U may be computed by Algorithm Polar; if either A or B is rank-deficient then U may be computed via a singular value decomposition of B^TA, as described in § 3.1 (see also [16, p. 426]).

6.2. Aerospace computations [2]-[7], [9], [28], [32]. In aerospace systems an important role is played by the direction cosine matrix (DCM)—an orthogonal matrix $D \in \mathbb{R}^{3\times 3}$ which transforms vectors from one coordinate system to another. Errors incurred in computation of the DCM result in a loss of orthogonality; an intuitively appealing way in which to restore orthogonality is to replace the computed DCM $\hat{D}$ by the nearest orthogonal matrix, that is, by the orthogonal polar factor of $\hat{D}$ (see Corollary 2.3).

A key feature of this application is that $\hat{D}$ is relatively close to being orthogonal: typically $\|\hat{D} - U\|_F < .1$ [2], [3], [4]. From (3.8) we can expect iteration (3.1) to converge within four iterations, for a tolerance $\delta_3 \geqq 10^{-16}$ in (3.17). Of course if U is not required to full machine accuracy then there is no need to iterate to convergence—just one or two iterations may yield a sufficiently accurate approximation to U.

For matrices that are as close to orthogonality as $\hat{D}$ above, computation of U from Algorithm Polar will require at most $4n^3$ flops, making this method particularly

attractive, since the singular value decomposition approach described in § 3.1 still requires approximately $12n^3$ flops.

We now compare Algorithm Polar with two other iterative techniques which have been proposed for computing the orthogonal polar factor of a nearly-orthogonal matrix.

Bjorck and Bowie [7] derive a family of iterative methods with orders of convergence $2, 3, \cdots$ by employing a binomial expansion for the matrix square root in the expression $U = AH^{-1} = A(A^*A)^{-1/2}$ (see Lemma 2.1(i)). Their quadratically convergent method is

$$X_0 = A, \tag{6.1a}$$

$$Q_k = I - X_k^* X_k, \tag{6.1b}$$

$$X_{k+1} = X_k(I + \tfrac{1}{2}Q_k), \qquad k = 0, 1, 2, \cdots. \tag{6.1c}$$

One step of this iteration costs $3n^3/2$ flops (for $A \in \mathbb{R}^{n\times n}$); in comparison iteration (3.1) requires only n^3 flops per step. Also, while iteration (3.1) converges for any nonsingular A, a practical condition for the convergence of iteration (6.1) is [7]

$$0 < \sigma_i(A) < \sqrt{3}, \qquad 1 \leqq i \leqq n.$$

The following iteration is proposed in [2]:

$$X_0 = A \in \mathbb{R}^{n\times n}, \tag{6.2a}$$

$$X_{k+1} = X_k - \tfrac{1}{2}(X_k A^T X_k - A), \qquad k = 0, 1, 2, \cdots. \tag{6.2b}$$

It is shown in [3], [5], [28] that iteration (6.2) is locally, linearly convergent to the orthogonal polar factor of A. Evaluation of iteration (6.2) requires $2n^3$ flops per step. Because of its linear convergence and its computational cost, this iteration is decidedly unattractive in comparison with iteration (3.1).

We appreciate that flop counts are not necessarily a fair means for comparing competing algorithms. In fact, because iterations (3.1), (6.1) and (6.2) use only matrix multiplications, inversions and additions, the flops involved in these iterations may be significantly cheaper than those in the Golub-Reinsch SVD algorithm, particularly on the new special computer architectures.

6.3. Optimisation. Newton's method for the minimisation of $F(x)$, $F: \mathbb{R}^n \to \mathbb{R}$, requires at each stage computation of a search direction p_k from

$$G_k p_k = -g_k,$$

where $g_k = \nabla F(x_k)$ is the gradient vector and

$$G_k = \left(\frac{\partial^2 F}{\partial x_i\, \partial x_j}(x_k)\right)$$

is the (symmetric) Hessian matrix. Difficulties occur when G_k is not positive definite since p_k, if defined, need not be a descent direction [14, p. 107]. We suggest that in this situation one replaces G_k by its polar factor H. H is positive definite (assuming G_k is nonsingular) and it has the properties listed in Lemmas 2.1 and 2.4. H may be computed using Algorithm Polar at a cost of $(s/2+1)n^3$ flops, if advantage is taken of the symmetry of the iterates (for example the LINPACK routine SSIDI [11] may be used to compute the matrix inverses). The equation $Hp_k = -g_k$ may be solved in $n^3/6$ flops by use of the Choleski decomposition.

In [14] several techniques are described for modifying G_k to give a related positive definite matrix. One of these consists of computing a spectral decomposition

$G_k = Z\Lambda Z^*$ and replacing G_k by $\hat{G}_k = Z|\Lambda|Z^*$; from (2.10) we recognize $\hat{G}_k$ as the polar factor H of G_k. This approach yields the same matrix as our suggestion, at a cost of about $6n^3$ flops [16, p. 282].

6.4. Matrix square root [8], [10], [20], [21], [25]. A new method for computing the symmetric positive definite square root $A^{1/2}$ of a symmetric positive definite matrix A is obtained from the observation that if

$$A = LL^T, \qquad L^T = UH$$

are Choleski and polar decompositions respectively, then (see Lemma 2.1(i)) $H = A^{1/2}$.

ALGORITHM ROOT. Given a symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$ this algorithm computes $A^{1/2}$.

(1) Compute the Choleski decomposition $A = LL^T$ [16, p. 89].

(2) Compute the Hermitian polar factor $H = A^{1/2}$ of L^T using Algorithm Polar.

Cost: $(s - \frac{1}{6})n^3$ flops, where s iterations of Algorithm Polar are required for convergence (taking into account the triangularity of L).

Note that since we are applying Algorithm Polar to L^T, the quantity $\kappa_2(A)$ in the bound (3.16) is replaced by $\kappa_2(L^T) = \kappa_2(A)^{1/2}$.

Algorithm Root is an attractive, numerically stable alternative (see § 5) to the iterations in [10], [21], [25] for the case where A is symmetric positive definite.

7. Numerical examples. In this section we present some test results which illustrate the performance of Algorithm Polar. The computations were performed using MATLAB [29] in double precision on a VAX 11/780 computer; the unit roundoff $u = 2^{-56} \approx 1.39 \times 10^{-17}$.

We used the convergence test (3.17) with $\delta_n = 4u$ for $n \leqq 25$ and $\delta_{50} = 8u$. Once the criterion $\|X_k - X_{k-1}\|_1 \leqq .01$ was satisfied $X_{k+1}, X_{k+2}, \cdots$ were computed using the unaccelerated iteration ($\gamma_j = 1, j > k$).

In the first test real matrices A of order $n = 5, 10, 25, 50$ were generated according to $A = U\Sigma V^T$, where $\Sigma = \operatorname{diag}(\sigma_i)$ is a matrix of singular values ($\sigma_i = i$, i^2, i^4 or 2^i) and U, V are random orthogonal matrices (different for each A), obtained from the QR decomposition of a matrix with elements from the uniform distribution on $[0, 1]$. The results are summarised in Table 7.1. The quantity

$$\text{BERR}_n = \frac{\|H_1 - H_1^*\|_1}{2\delta_n \|A\|_1}$$

is the backward error measure derived in § 4 (see (4.1b)) and must be of order one for the algorithm to have performed in a stable manner. For every matrix in this test the computed Hermitian polar factor $\hat{H}$ was positive definite.

TABLE 7.1
Number of iterations.

	$n = 5$	10	25	50
$\sigma_i = i$	6	7	8	8
$\sigma_i = i^2$	7	7	10	9
$\sigma_i = i^4$	8	8	10	10
$\sigma_i = 2^i$	7	8	9	10
max BERR_n	.38	.55	2.1	2.8

The second test compares Algorithm Polar with iterations (6.1) and (6.2) (using the same convergence test, (3.17), for each iteration). The parametrised matrix

$$A(\alpha)=\begin{pmatrix} \alpha & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

is orthogonal for $\alpha = 0$. The results are displayed in Table 7.2.

TABLE 7.2
Number of iterations.

α	Algorithm Polar	Iteration (6.1)	Iteration (6.2)
.001	4	4	5
.01	4	4	8
.1	5	5	13
1	6	10	76
2	7	diverged	diverged

8. Conclusions. From the test results of § 7 and the theory of § 3 we draw several conclusions about Algorithm Polar.

The acceleration parameter estimates are very effective. Convergence to a tolerance $\delta_n \leqq 10^{-17}$ (see (3.17)) is usually obtained within ten iterations, the computational cost of one iteration being approximately n^3 flops.

In applications where A is nearly orthogonal (see § 6.2) Algorithm Polar is an attractive alternative to iterations (6.1) and (6.2)—it is guaranteed to converge (within four or five iterations, typically) and it will usually be computationally the least expensive of the three methods.

We have not proved that Algorithm Polar is stable, that is, that the computed polar factors are relatively close to the true polar factors of a matrix near to A. The tests (4.1) provide an inexpensive means of monitoring the stability of Algorithm Polar. Algorithm Polar has performed stably in all our numerical tests, producing, in every case, computed polar factors which are just as acceptable as those furnished by the SVD approach.

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