SIAM J. Matrix Anal. Appl.
Vol. 37, No. 4, pp. 1453–1477

MATRIX INVERSE TRIGONOMETRIC AND INVERSE HYPERBOLIC FUNCTIONS: THEORY AND ALGORITHMS*

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Abstract. Theoretical and computational aspects of matrix inverse trigonometric and inverse hyperbolic functions are studied. Conditions for existence are given, all possible values are characterized, and the principal values acos, asin, acosh, and asinh are defined and shown to be unique primary matrix functions. Various functional identities are derived, some of which are new even in the scalar case, with care taken to specify precisely the choices of signs and branches. New results include a "round trip" formula that relates $\operatorname{acos}(\cos A)$ to A and similar formulas for the other inverse functions. Key tools used in the derivations are the matrix unwinding function and the matrix sign function. A new inverse scaling and squaring type algorithm employing a Schur decomposition and variable-degree Padé approximation is derived for computing acos, and it is shown how it can also be used to compute asin, acosh, and asinh. In numerical experiments the algorithm is found to behave in a forward stable fashion and to be superior to computing these functions via logarithmic formulas.

Key words. matrix function, inverse trigonometric functions, inverse hyperbolic functions, matrix inverse sine, matrix inverse cosine, matrix inverse hyperbolic sine, matrix inverse hyperbolic cosine, matrix exponential, matrix logarithm, matrix sign function, rational approximation, Padé approximation, MATLAB, GNU Octave, Fréchet derivative, condition number

AMS subject classifications. 15A24, 65F30

DOI. 10.1137/16M1057577

1. Introduction.

Trigonometric functions of matrices play an important role in the solution of second order differential equations; see, for example, [5], [37], and the references therein. The inverses of such functions, and of their hyperbolic counterparts, also have practical applications, but have been less well studied. An early appearance of the matrix inverse cosine was in a 1954 paper on the energy equation of a free-electron model [36]. The matrix inverse hyperbolic sine arises in a model of the motion of rigid bodies, expressed via Moser–Veselov matrix equations [12]. The matrix inverse sine and inverse cosine were used by Al-Mohy, Higham, and Relton [5] to define the backward error in approximating the matrix sine and cosine. Matrix inverse trigonometric and inverse hyperbolic functions are also useful for studying argument reduction in the computation of the matrix sine, cosine, and hyperbolic sine and cosine [7].

This work has two aims. The first is to develop the theory of matrix inverse trigonometric functions and inverse hyperbolic functions. Most importantly, we define the principal values acos, asin, acosh, and asinh, prove their existence and uniqueness, and develop various useful identities involving them. In particular, we determine the precise relationship between $\operatorname{acos}(\cos A)$ and A, and similarly for the other functions. The second aim is to develop algorithms and software for computing acos, asin, acosh, and asinh of a matrix, for which we employ variable-degree Padé approximation to-

*Received by the editors January 20, 2016; accepted for publication (in revised form) by C.-H. Guo August 1, 2016; published electronically October 11, 2016.

http://www.siam.org/journals/simax/37-4/M105757.html

Funding: This work was supported by European Research Council Advanced Grant MATFUN (267526). The work of the second author was also supported by Engineering and Physical Sciences Research Council grant EP/I01912X/1.

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gether with appropriate initial transformations. Very little has been published on computation of these matrix functions, and the only publicly available software we are aware of that is designed specifically for computing these functions is in GNU Octave [18], [23].

Corless et al. [15] note that in the elementary function literature, definitions and identities are often imprecise or inconsistent and need careful interpretation. While it is arguably reasonable to ask a reader to determine the correct sign or choice of branch in a scalar formula, in a formula in $n \times n$ matrices, whose information content is at least n scalar identities involving the (unknown) eigenvalues, imprecision is a recipe for confusion and controversy. We are therefore scrupulous in this work to give precise definitions and derive formulas that are valid under clearly stated conditions.

In section 2 we give necessary and sufficient conditions for the existence of matrix inverse cosine and sine functions and their hyperbolic counterparts and characterize all their possible values. Then we define the branch points, branch cuts, and principal values and prove the uniqueness of the principal values. In section 3 we develop a variety of identities involving the matrix inverse functions, some of which are new even in the scalar case. In section 4 we discuss the conditioning of the inverse functions. An algorithm for computing acos that combines a Schur decomposition and Padé approximation with a square root recurrence is given in section 5; the algorithm yields algorithms for asin, acosh, and sinh. In section 6 we give numerical experiments that compare the new algorithms with the use of formulas based on the matrix logarithm and square root. Concluding remarks are given in section 7.

2. The inverse functions.

We first define and characterize the matrix inverse trigonometric and inverse hyperbolic functions and then treat their principal values. We will repeatedly use the principal matrix logarithm, principal matrix square root, and matrix sign function, with extensions on their respective branch cuts. These are defined as follows.

A logarithm of a nonsingular $A \in \mathbb{C}^{n\times n}$, written $X = \operatorname{Log} A$, is a solution of $\mathrm{e}^X = A$. The principal logarithm of a nonsingular $A \in \mathbb{C}^{n\times n}$, denoted $\log A$, is the logarithm all of whose eigenvalues have imaginary parts in the interval $(-\pi, \pi]$. We take the branch cut to be the negative real axis $\mathbb{R}^-$. Note that the principal matrix logarithm is usually not defined for matrices with eigenvalues on the negative real axis [21, Chap. 11], but for the purposes of this work it is convenient to allow the extension of the logarithm on the branch cut and to adopt the convention that $\log(-y) = \log y + \pi\mathrm{i}$ for $y > 0$.

A square root of $A \in \mathbb{C}^{n\times n}$, written $X = \sqrt{A}$, is a solution of $X^2 = A$. We take the branch cut to be $\mathbb{R}^-$ and define the principal square root to be the one all of whose eigenvalues have nonnegative real parts and such that $(-y)^{1/2} = y^{1/2}\mathrm{i}$ for $y > 0$. Consistent with the principal logarithm defined above, we can write the principal square root of any nonsingular complex matrix A as $A^{1/2} = \mathrm{e}^{\frac{1}{2}\log A}$.

We also need the matrix sign function $\operatorname{sign} A$ [21, Chap. 5], which maps each eigenvalue of A to the sign (± 1) of its real part. To include the case where A has an eigenvalue on the imaginary axis, we define $\operatorname{sign}(0) = 1$ and $\operatorname{sign}(y\mathrm{i}) = \operatorname{sign}(y)$ for nonzero $y \in \mathbb{R}$.

These particular choices for the values of the sign function and the logarithm and square root on their branch cuts, which we previously used in [6], adhere to the counterclockwise continuity principle introduced by Kahan [27, sect. 5].

We recall that for a multivalued function f a nonprimary matrix function $f(A)$ is obtained if, in the definition of matrix function via the Jordan canonical form, some eigenvalue λ appears in more than one Jordan block and is assigned different values $f(\lambda)$ on at least two of the blocks [21, sect. 1.2]. This means that $f(A)$ is not expressible as a polynomial in A.

2.1. Existence and characterization. An inverse cosine of $A \in \mathbb{C}^{n\times n}$ is any solution of the equation $\cos X = A$. Inverse sines, and inverse hyperbolic sines and cosines, are defined in an analogous way.

Using Euler's formula, for $X \in \mathbb{C}^{n\times n}$,

$$\mathrm{e}^{\mathrm{i}X} = \cos X + \mathrm{i}\sin X, \tag{2.1}$$

we can write the matrix cosine and sine functions in their exponential forms

$$\cos X = \frac{\mathrm{e}^{\mathrm{i}X} + \mathrm{e}^{-\mathrm{i}X}}{2}, \qquad \sin X = \frac{\mathrm{e}^{\mathrm{i}X} - \mathrm{e}^{-\mathrm{i}X}}{2\mathrm{i}}. \tag{2.2}$$

To establish whether solutions to the equation $A = \cos X$ exist we use the exponential form to write $A = (\mathrm{e}^{\mathrm{i}X} + \mathrm{e}^{-\mathrm{i}X})/2$. This equation implies that A commutes with the nonsingular matrix $\mathrm{e}^{\mathrm{i}X}$, and after multiplying through by $\mathrm{e}^{\mathrm{i}X}$ the equation can be written as

$$(\mathrm{e}^{\mathrm{i}X} - A)^2 = A^2 - I.$$

Taking square roots gives

$$\mathrm{e}^{\mathrm{i}X} = A + \sqrt{A^2 - I}, \tag{2.3}$$

provided that $A^2 - I$ has a square root. The matrix $A + \sqrt{A^2 - I}$ is always nonsingular, and so we can take logarithms to obtain $X = -\mathrm{i}\,\mathrm{Log}(A + \sqrt{A^2 - I})$. Any inverse matrix cosine must have this form. In order to reverse the steps of this argument we need to show that $\mathrm{e}^{\mathrm{i}X}$ commutes with A, which can be guaranteed when $\sqrt{A^2 - I}$ can be expressed as a polynomial in A, which in turn is true if the square root is a primary matrix function [21, sect. 1.2], that is, if each occurrence of any repeated eigenvalue is mapped to the same square root. If a nonprimary square root is taken it may or may not yield an inverse cosine.

Similar analysis can be done for the matrix inverse sine. Results for the inverse hyperbolic functions can be obtained using the relations

$$\cosh X = \cos \mathrm{i}X, \qquad \sinh X = -\mathrm{i}\sin \mathrm{i}X, \tag{2.4}$$

which hold for any $X \in \mathbb{C}^{n\times n}$ and can be taken as the definitions of cosh and sinh.

THEOREM 2.1. *Let $A \in \mathbb{C}^{n\times n}$.*

(a) *The equation $\cos X = A$ has a solution if and only if $A^2 - I$ has a square root. Every solution has the form $X = -\mathrm{i}\,\mathrm{Log}(A + \sqrt{A^2 - I})$ for some square root and logarithm.*

(b) *The equation $\sin X = A$ has a solution if and only if $I - A^2$ has a square root. Every solution has the form $X = -\mathrm{i}\,\mathrm{Log}(\mathrm{i}A + \sqrt{I - A^2})$ for some square root and logarithm.*

(c) *The equation $\cosh X = A$ has a solution if and only if $A^2 - I$ has a square root. Every solution has the form $X = \mathrm{Log}(A + \sqrt{A^2 - I})$ for some square root and logarithm.*

(d) *The equation $\sinh X = A$ has a solution if and only if $A^2 + I$ has a square root. Every solution has the form $X = \mathrm{Log}(A + \sqrt{A^2 + I})$ for some square root and logarithm.*

In (a)–(d) *the given expression for X is guaranteed to be a solution when the square root is a primary square root.*

We emphasize that the square roots and logarithms in the statement of the theorem need not be primary. Note also that the existence of a square root of a matrix is in question only when the matrix is singular. Necessary and sufficient conditions for the existence of a square root of a singular matrix are given in [16], [21, Thm. 1.22].

To illustrate the use of these results, we consider the existence of an inverse sine of the 2×2 matrix $A = \left[\begin{smallmatrix} 1 & 1996 \\ 0 & 1 \end{smallmatrix}\right]$ [21, Prob. 1.50] (Putnam Problem 1996–B4). It is easy to see that $I - A^2 = \left[\begin{smallmatrix} 0 & -3992 \\ 0 & 0 \end{smallmatrix}\right]$ does not have a square root, and hence the equation $A = \sin X$ has no solutions. Two very similar 2×2 examples are given by Pólya and Szegö [35, Prob. 210, p. 35].

2.2. Branch points, branch cuts, and principal values. The inverse cosine and inverse sine functions, and their hyperbolic counterparts, are multivalued. We now specify their branch points and branch cuts. The branch points of acos and asin are at 1 and -1 and, in accordance with popular convention [32, sects. 4.23(ii), 4.23(vii)], we consider their branch cuts to be on the two segments of the real line

$$\Omega = \Omega_1 \cup \Omega_2 = (-\infty, -1] \cup [1, \infty). \tag{2.5}$$

The branch points of asinh are at i and $-$i, and the branch cuts are the segments of the imaginary line iΩ; the branch points of acosh are at 1 and -1, and the branch cut is the segment of the real line [32, sect. 4.37(ii)]

$$\widetilde{\Omega} = \Omega_1 \cup \Omega_3 \equiv (-\infty, -1] \cup [-1, 1] = (-\infty, 1]. \tag{2.6}$$

In the following definition we specify the principal values of the functions, in a way consistent with the scalar case [32, sects. 4.23(ii), 4.37(ii)] and with the counterclockwise continuity principle [27]. We refer the reader to Figure 2.1 for plots of the domains and ranges of the principal branches of the scalar functions (the plots extend ones in [34]). The figure also shows where the branch cuts are and what values the principal functions take on these branch cuts. The hashes placed on the sides of the branch cuts indicate that if a sequence $\{z_k\}$ tends to a point w on the branch cut from the side with the hashes then $\lim_{k\to\infty} f(z_k) \neq f(w)$.

Definition 2.2 (principal values). *Let $A \in \mathbb{C}^{n\times n}$.*

(a) *The principal inverse cosine of A, denoted* acos$A$*, is the inverse cosine for which every eigenvalue*
   (i) *has real part lying in $(0, \pi)$, or*
   (ii) *has zero real part and nonnegative imaginary part* (*corresponding to A having an eigenvalue in Ω_2*)*, or*
   (iii) *has real part π and nonpositive imaginary part* (*corresponding to A having an eigenvalue in Ω_1*)*.*

(b) *The principal inverse sine of A, denoted* asin$A$*, is the inverse sine for which every eigenvalue*
   (i) *has real part lying in $(-\pi/2, \pi/2)$, or*
   (ii) *has real part $-\pi/2$ and nonnegative imaginary part* (*corresponding to A having an eigenvalue in Ω_1*)*, or*
   (iii) *has real part $\pi/2$ and nonpositive imaginary part* (*corresponding to A having an eigenvalue in Ω_2*)*.*

(c) *The principal inverse hyperbolic cosine of A, denoted* acosh$A$*, is the inverse hyperbolic cosine for which every eigenvalue*

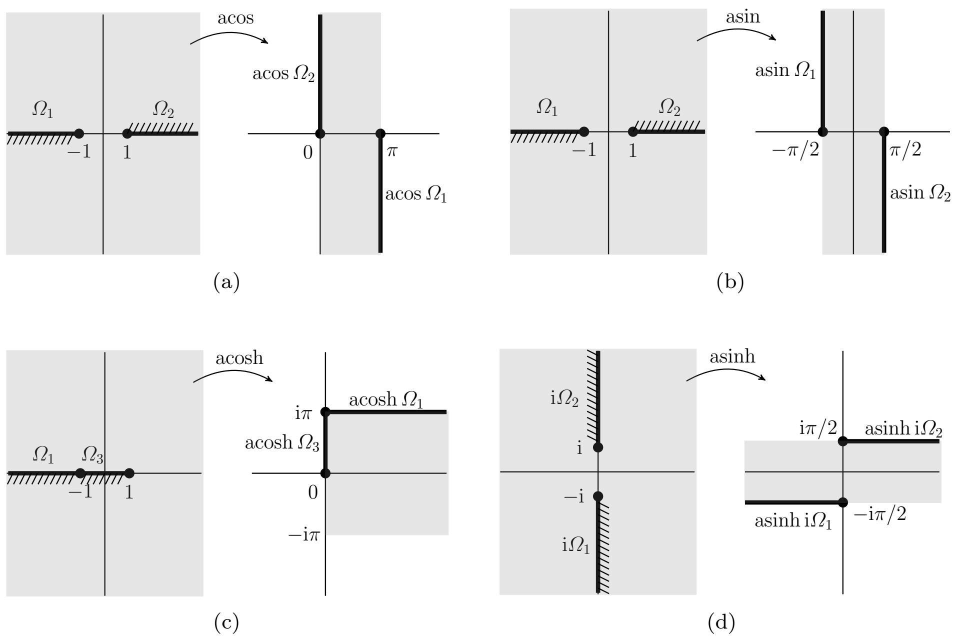

FIG. 2.1. *Domains and ranges of the principal branches of the complex functions* acos (a), asin (b), acosh (c), and asinh (d).

(i) *has imaginary part lying in* $(-\pi, \pi)$ *and positive real part, or*
(ii) *has imaginary part in* $[0, \pi)$ *and zero real part* (*corresponding to* A *having an eigenvalue in* Ω_3), *or*
(iii) *has imaginary part* π *and nonnegative real part* (*corresponding to* A *having an eigenvalue in* Ω_1).

(d) *The principal inverse hyperbolic sine of* A*, denoted* $\operatorname{asinh} A$*, is the inverse hyperbolic sine for which every eigenvalue*
(i) *has imaginary part lying in* $(-\pi/2, \pi/2)$*, or*
(ii) *has imaginary part* $-\pi/2$ *and nonpositive real part* (*corresponding to* A *having an eigenvalue in* $\mathrm{i}\Omega_1$), *or*
(iii) *has imaginary part* $\pi/2$ *and nonnegative real part* (*corresponding to* A *having an eigenvalue in* $\mathrm{i}\Omega_2$).

Note that if A has no eigenvalues on the respective branch cuts then part (i) of each of (a)–(d) in Definition 2.2 is in operation. Moreover, under this condition the principal inverse function exists, is unique, and is a primary matrix function of A, as shown by the next result.

THEOREM 2.3. *Let* $A \in \mathbb{C}^{n\times n}$.
(a) *If* A *has no eigenvalues equal to* 1 *or* -1 *then there is a unique principal inverse cosine* $\operatorname{acos} A$*, a unique principal inverse sine* $\operatorname{asin} A$*, and a unique principal inverse hyperbolic cosine* $\operatorname{acosh} A$*, and all are primary matrix functions of* A.
(b) *If* A *has no eigenvalues equal to* i *or* $-\mathrm{i}$ *then there is a unique principal inverse hyperbolic sine* $\operatorname{asinh} A$ *and it is a primary matrix function of* A.

Proof. Consider asin, which by Definition 2.2 must have eigenvalues with real parts in the interval $(-\pi/2, \pi/2)$, or real parts $-\pi/2$ and nonnegative imaginary parts, or real parts $\pi/2$ and nonpositive imaginary parts. Note first that inverse sines exist by Theorem 2.1 (b), since $I - A^2$ is nonsingular under the assumptions on A. Observe that a nonprimary inverse sine of A (if one exists) must have two eigenvalues μ_i and μ_j with $\mu_j = (-1)^k\mu_i + k\pi$ for some nonzero integer k. Since A has no eigenvalues equal to 1 or -1 such an inverse sine cannot satisfy Definition 2.2 (b). Therefore no nonprimary inverse sine can be a principal inverse sine. Finally, there exists a way, and hence precisely one way, to map the eigenvalues with the inverse sine in such a way that all eigenvalues have the characterization given in Definition 2.2, and that is with asin.

The proofs for acos, acosh, and asinh are completely analogous. □

3. Identities. Now we derive identities involving the principal matrix inverse trigonometric and inverse hyperbolic functions. Some of the results generalize existing scalar results, but others are new even in the scalar case.

The first result provides explicit formulas for the principal inverse functions in terms of the principal logarithm and the principal square root. Note that the exclusion of the branch points as eigenvalues of A in the next result, and in later results, is necessary in order to ensure the existence of the inverse functions.

THEOREM 3.1. *For $A \in \mathbb{C}^{n\times n}$, assuming that A has no eigenvalues at the branch points of the respective inverse functions,*

$$\begin{aligned} \text{acos} A &= -\mathrm{i}\log(A + \mathrm{i}(I - A^2)^{1/2}) \\ &= -2\mathrm{i}\log\left(\left(\frac{I+A}{2}\right)^{1/2} + \mathrm{i}\left(\frac{I-A}{2}\right)^{1/2}\right), \end{aligned} \tag{3.1}$$

$$\text{asin} A = -\mathrm{i}\log(\mathrm{i}A + (I - A^2)^{1/2}), \tag{3.2}$$

$$\begin{aligned} \text{acosh} A &= \log(A + (A - I)^{1/2}(A + I)^{1/2}) \\ &= 2\log\left(\left(\frac{A+I}{2}\right)^{1/2} + \left(\frac{A-I}{2}\right)^{1/2}\right), \end{aligned} \tag{3.3}$$

$$\text{asinh} A = \log(A + (A^2 + I)^{1/2}). \tag{3.4}$$

Proof. These identities are known to hold for complex scalars [14], [27], [32, sects. 4.23(iv), 4.37(iv)], and the formula (3.4) is given in [10] under different assumptions on A. If we were to exclude the eigenvalues of A from the branch cuts, which are the only points of nondifferentiability of the inverse functions, it would follow from [21, Thm. 1.20], [25, Thm. 6.2.27 (2)] that the identities hold in the matrix case. In fact, they hold even if A has eigenvalues on the branch cuts. We show only that the first equality in (3.1) holds, as the proofs of the remaining identities are analogous. From the given conditions, the matrix $-\mathrm{i}\log(A + \mathrm{i}(I - A^2)^{1/2})$ exists and by Theorem 2.1 (a) it is an inverse cosine of A. It is readily verified that the eigenvalues of $-\mathrm{i}\log(A+\mathrm{i}(I-A^2)^{1/2})$ satisfy the conditions of Definition 2.2 (a), and therefore $-\mathrm{i}\log(A + \mathrm{i}(I - A^2)^{1/2})$ must be the principal inverse cosine of A. □

The next result completely describes the relation between the acos and asin functions. It is the matrix counterpart of [32, eq. (4.23.16)].

LEMMA 3.2. *If $A \in \mathbb{C}^{n\times n}$ has no eigenvalues ± 1 then*

$$\text{acos} A + \text{asin} A = \frac{\pi}{2} I. \tag{3.5}$$

Proof. Using the addition formula for the cosine we find that $\cos(\frac{\pi}{2}I - \operatorname{asin} A) = A$, so $\frac{\pi}{2}I - \operatorname{asin} A$ is some inverse cosine of A. That it is the principal inverse cosine is easily seen from Definition 2.2 (a) and (b). ∎

A known identity for scalars is $\operatorname{acosh} z = \pm\mathrm{i} \operatorname{acos} z$ [1, eq. (4.6.15)]. The correct choice of sign depends on the complex argument of $1 - z$ (see Corless et al. [15, sect. 6.2]). In the next result we show that the ± 1 term can be explicitly expressed in terms of the sign function and generalize the identity to matrices. We also generalize a corresponding identity for asinh.

THEOREM 3.3. *If $A \in \mathbb{C}^{n\times n}$ has no eigenvalues ± 1 then*

$$\operatorname{acosh} A = \mathrm{i} \operatorname{sign}(-\mathrm{i}A) \operatorname{acos} A \quad \textit{if } A \textit{ has no eigenvalues in } (0,1], \tag{3.6}$$

$$\operatorname{asinh}(\mathrm{i}A) = \mathrm{i} \operatorname{asin} A. \tag{3.7}$$

Proof. From (2.4) along with the fact that cosh is an even function, we see that if X is an inverse cosine of A then $\pm\mathrm{i}X$ is an inverse hyperbolic cosine of A. By passing to the Jordan canonical form and applying the argument to each Jordan block, it follows that $\mathrm{i} \operatorname{sign}(-\mathrm{i}A) \operatorname{acos} A$ is some hyperbolic inverse cosine of A, and we need to show that it is the principal hyperbolic inverse cosine. We therefore need to show that the eigenvalues of $\mathrm{i} \operatorname{sign}(-\mathrm{i}A) \operatorname{acos} A$ satisfy the conditions in Definition 2.2 (c), which is equivalent to showing that $\mathrm{i} \operatorname{sign}(-\mathrm{i}z) \operatorname{acos} z$ satisfies these conditions for all $z \in \mathbb{C} \setminus (0, 1]$.

Write $\operatorname{acos} z = x + \mathrm{i}y$, where $z \in \mathbb{C}$ and $x, y \in \mathbb{R}$. We can also write $z = \cos(x + \mathrm{i}y)$, which, using the addition formula for cosine, we can expand to $z = \cos x \cos(\mathrm{i}y) - \sin x \sin(\mathrm{i}y)$. Assuming that $y \neq 0$ and $x \in (0, \pi)$, we have $\operatorname{sign}(-\mathrm{i}z) = \operatorname{sign}(\mathrm{i} \sin x \sin(\mathrm{i}y))$, because $\cos x$, $\sin x$, and $\cos(\mathrm{i}y)$ are all real, and $\sin(\mathrm{i}y)$ is pure imaginary. Since $x \in (0, \pi)$, $\sin x > 0$, and $\sin(\mathrm{i}y) = \mathrm{i} \sinh y$, we have $\operatorname{sign}(-\mathrm{i}z) = \operatorname{sign}(-\sinh y) = -\operatorname{sign} y$. Finally, $\mathrm{i} \operatorname{sign}(-\mathrm{i}z) \operatorname{acos} z = -\mathrm{i} \operatorname{sign}(y)(x + \mathrm{i}y)$, which has real part $y \operatorname{sign} y > 0$ and imaginary part $-x \operatorname{sign} y \in (-\pi, \pi)$, satisfying Definition 2.2 (c) (i). If $y = 0$ then $z \in (-1, 1)$, and now we consider in turn $z \in (-1, 0]$ and $z \in (0, 1)$. In the former case, $x \in [\pi/2, \pi)$, and so $\mathrm{i} \operatorname{sign}(-\mathrm{i}z) \operatorname{acos} z \in \mathrm{i}[\pi/2, \pi)$. In the other case, $x \in (0, \pi/2)$, and so $\mathrm{i} \operatorname{sign}(-\mathrm{i}z) \operatorname{acos} z \in \mathrm{i}(-\pi/2, 0)$, which is not in the range of the principal branch of acosh. This means that Definition 2.2 (c) (ii) is satisfied for $z \in (-1, 0]$, but it is not satisfied for $z \in (0, 1)$. If $x = 0$, by Definition 2.2 (a) (ii) we have $y > 0$, and so $z > 1$ and $\mathrm{i} \operatorname{sign}(-\mathrm{i}z) \operatorname{acos} z = y$, which satisfies Definition 2.2 (c) (i). Similarly, if $x = \pi$ then $y < 0$ by Definition 2.2 (a) (iii), and so $z < -1$ and $\mathrm{i} \operatorname{sign}(-\mathrm{i}z) \operatorname{acos} z = -y + \pi\mathrm{i}$, which satisfies Definition 2.2 (c) (iii).

Turning to (3.7), from (2.4) we see that if X is an inverse sine of A then $\mathrm{i}X$ is some inverse hyperbolic sine of $\mathrm{i}A$. We therefore just need to check that $\mathrm{i} \operatorname{asin} A$ is the principal inverse hyperbolic sine of $\mathrm{i}A$, and this reduces to the scalar case, which is a known identity [1, eq. (4.6.14)]. ∎

For the next results we need to introduce the matrix unwinding function [6], which is defined for any $A \in \mathbb{C}^{n\times n}$ by

$$\mathcal{U}(A) = \frac{A - \log \mathrm{e}^A}{2\pi\mathrm{i}}, \tag{3.8}$$

where log is the principal matrix logarithm defined at the beginning of section 2. The following characterization of when the matrix unwinding function is zero, from [6, Thm. 3.1], will be used several times.

LEMMA 3.4. *For $A \in \mathbb{C}^{n\times n}$, $\mathcal{U}(A) = 0$ if and only if the imaginary parts of all the eigenvalues of A lie in the interval $(-\pi, \pi]$.*

To prove the following identities we also need the next result, which generalizes a result for scalars in [9, Lem. 2].

LEMMA 3.5. *For $A \in \mathbb{C}^{n\times n}$ with no eigenvalues ± 1,*

$$(I - A)^{1/2}(I + A)^{1/2} = (I - A^2)^{1/2}. \tag{3.9}$$

Moreover, if all the eigenvalues of A have arguments in the interval $(-\pi/2, \pi/2]$ then

$$(A - I)^{1/2}(A + I)^{1/2} = (A^2 - I)^{1/2}. \tag{3.10}$$

Proof. Using the fact that $\log(I - A)$ and $\log(A + I)$ commute, together with [6, Lem. 3.12], we have

$$\begin{aligned}(I - A)^{1/2}(I + A)^{1/2} &= \mathrm{e}^{\frac{1}{2}\log(I-A)}\mathrm{e}^{1/2\log(I+A)} \\ &= \mathrm{e}^{\frac{1}{2}(\log(I-A)+\log(I+A))} \\ &= \mathrm{e}^{\frac{1}{2}(\log(I-A^2)+2\pi\mathrm{i}\,\mathcal{U}(\log(I-A)+\log(I+A)))}.\end{aligned}$$

It is easy to show, as in the proof of [9, Lem. 2], that $\mathrm{Im}[\log(1-z)+\log(1+z)] \in (-\pi, \pi]$ for all $z \in \mathbb{C}$, and in particular for all the eigenvalues of A, and by Lemma 3.4 it follows that $\mathcal{U}(\log(I - A) + \log(I + A)) = 0$. Therefore $(I - A)^{1/2}(I + A)^{1/2} = \mathrm{e}^{\frac{1}{2}\log(I-A^2)} = (I - A)^{1/2}$. The proof of (3.10) is analogous. □

We emphasize that, unlike (3.9), the identity (3.10) does not hold for all matrices A for which ± 1 is outside the spectrum.

The formulas in the next result will be useful in the construction of algorithms for computing acos, asin, acosh, and asinh in section 5. These formulas do not follow directly from the scalar addition formulas in [32, sects. 4.24(iii), 4.38(iii)] because the latter formulas do not specify the branches of the constituent terms.

THEOREM 3.6. *For $A \in \mathbb{C}^{n\times n}$, assuming that A has no eigenvalues at the branch points of the respective functions,*

$$\operatorname{acos} A = 2\operatorname{acos}\left(\left(\frac{I + A}{2}\right)^{1/2}\right), \tag{3.11}$$

$$\operatorname{asin} A = 2\operatorname{asin}\left(\frac{(I + A)^{1/2} - (I - A)^{1/2}}{2}\right), \tag{3.12}$$

$$\operatorname{acosh} A = 2\operatorname{acosh}\left(\left(\frac{I + A}{2}\right)^{1/2}\right), \tag{3.13}$$

$$\operatorname{asinh} A = 2\operatorname{asinh}\left(\frac{\mathrm{i}(I - \mathrm{i}A)^{1/2} - \mathrm{i}(I + \mathrm{i}A)^{1/2}}{2}\right). \tag{3.14}$$

Proof. To prove (3.11) we use the first and second logarithmic representations

(3.1) of acos, in that order:

$$\begin{aligned}
2\,\mathrm{acos}\left(\left(\frac{I+A}{2}\right)^{1/2}\right) &= -2\mathrm{i}\log\left(\left(\frac{I+A}{2}\right)^{1/2} + \mathrm{i}\left(I - \frac{I+A}{2}\right)^{1/2}\right)\\
&= -2\mathrm{i}\log\left(\left(\frac{I+A}{2}\right)^{1/2} + \mathrm{i}\left(\frac{I-A}{2}\right)^{1/2}\right)\\
&= \mathrm{acos} A.
\end{aligned}$$

The proof of (3.13) is analogous to that of (3.11) but requires the use of

$$\left(\left(\frac{I+A}{2}\right)^{1/2} - I\right)^{1/2}\left(\left(\frac{I+A}{2}\right)^{1/2} + I\right)^{1/2} = \left(\frac{I+A}{2} - I\right)^{1/2}.$$

The latter equality is valid by Lemma 3.5, since $((I+A)/2)^{1/2}$ has eigenvalues with arguments in the interval $(-\pi/2, \pi/2]$ by the definition of the principal square root.

For the proof of (3.12) we use the logarithmic representation (3.2) of asin. Denoting $B = ((I+A)^{1/2} - (I-A)^{1/2})/2$, after some manipulations we have $\mathrm{i}A + (I - A^2)^{1/2} = (\mathrm{i}B + (I - B^2)^{1/2})^2$. It is straightforward to show that for any $z \in \mathbb{C}$, $\mathrm{Re}(\mathrm{i}z \ + (1-z^2)^{1/2}) \geq 0$, from which we can conclude that $(\mathrm{i}A + (I-A^2)^{1/2})^{1/2} = \mathrm{i}B + (I - B^2)^{1/2}$. Taking logarithms, and using [6, Cor. 3.10],

$$\begin{aligned}
\frac{1}{2}\,\mathrm{asin} A &= -\frac{1}{2}\mathrm{i}\log(\mathrm{i}A + (I-A^2)^{1/2})\\
&= -\mathrm{i}\log(\mathrm{i}B + (I-B^2)^{1/2})\\
&= \mathrm{asin} B,
\end{aligned}$$

which is (3.12). To show that (3.14) holds, we use (3.12) and the relation (3.7) between asin and asinh. ∎

We will also use the formulas in the next result, which relate the trigonometric functions cos and sin and their inverses acos and asin, and generalize formulas for scalars in [32, Table 4.16.3].

LEMMA 3.7. *If $A \in \mathbb{C}^{n\times n}$ has no eigenvalues ± 1 then*

$$\sin(\mathrm{acos} A) = \cos(\mathrm{asin} A) = (I - A^2)^{1/2}.$$

Proof. Using the exponential form (2.2) of the sine and the logarithmic representation of acos given in Theorem 3.1, we write

$$\begin{aligned}
\sin(\mathrm{acos} A) &= \frac{\mathrm{e}^{\mathrm{i}\,\mathrm{acos} A} - (\mathrm{e}^{\mathrm{i}\,\mathrm{acos} A})^{-1}}{2i}\\
&= \frac{A + \mathrm{i}(I-A^2)^{1/2} - \big(A + \mathrm{i}(I-A^2)^{1/2}\big)^{-1}}{2\mathrm{i}}.
\end{aligned}$$

But $(A + \mathrm{i}(I-A^2)^{1/2})^{-1} = A - \mathrm{i}(I-A^2)^{1/2}$, so

$$\sin(\mathrm{acos} A) = \frac{A + \mathrm{i}(I-A^2)^{1/2} - \big(A - \mathrm{i}(I-A^2)^{1/2}\big)}{2\mathrm{i}} = (I-A^2)^{1/2}.$$

In a similar way, it can be shown that $\cos(\mathrm{asin} A) = (I-A^2)^{1/2}$. ∎

We now give summation formulas for the principal inverse sine and cosine functions. These identities are known to hold for real scalars, but by using the matrix unwinding function we can generalize them to complex square matrices.

In the remaining results of this section we make assumptions that are stronger than A having no eigenvalues at the branch points of the respective inverse functions. This is done so that we can obtain necessary and sufficient conditions for identities to hold.

The first result is given for scalars in [32, eq. (4.24.13)] for the multivalued inverse sine, with the branch for each occurrence of an inverse sine not specified.

THEOREM 3.8. *For all $A, B \in \mathbb{C}^{n\times n}$ with no eigenvalues in Ω and such that $AB = BA$,*

$$\operatorname{asin} A + \operatorname{asin} B = \operatorname{asin}\bigl(A(I-B^2)^{1/2} + B(I-A^2)^{1/2}\bigr)$$

if and only if all the eigenvalues of $-AB + (I-A^2)^{1/2}(I-B^2)^{1/2}$ have arguments in the interval $(-\pi/2, \pi/2]$.

Proof. Applying the logarithmic representation (3.2) and the formula describing the logarithm of a matrix product via the unwinding function [6, Lem. 3.12], we have

$$\begin{aligned}
\operatorname{asin} A + \operatorname{asin} B &= -\mathrm{i}\log\bigl(\mathrm{i}A + (I-A^2)^{1/2}\bigr) - \mathrm{i}\log\bigl(\mathrm{i}B + (I-B^2)^{1/2}\bigr)\\
&= -\mathrm{i}\log\bigl(\bigl(\mathrm{i}A + (I-A^2)^{1/2}\bigr)\bigl(\mathrm{i}B + (I-B^2)^{1/2}\bigr)\bigr)\\
&\quad + 2\pi\,\mathcal{U}\bigl(\log\bigl(\mathrm{i}A + (I-A^2)^{1/2}\bigr) + \log\bigl(\mathrm{i}B + (I-B^2)^{1/2}\bigr)\bigr)\\
&= -\mathrm{i}\log\bigl(\bigl(\mathrm{i}A + (I-A^2)^{1/2}\bigr)\bigl(\mathrm{i}B + (I-B^2)^{1/2}\bigr)\bigr)\\
&\quad + 2\pi\,\mathcal{U}\bigl(\mathrm{i}\operatorname{asin} A + \mathrm{i}\operatorname{asin} B).
\end{aligned}$$

Expanding the product and rearranging, using the fact that A and B commute, gives

$$\bigl(\mathrm{i}A + (I-A^2)^{1/2}\bigr)\bigl(\mathrm{i}B + (I-B^2)^{1/2}\bigr) = \mathrm{i}C - AB + (I-A^2)^{1/2}(I-B^2)^{1/2},$$

where $C = A(I-B^2)^{1/2} + B(I-A^2)^{1/2}$. We also note that

$$\bigl(-AB + (I-A^2)^{1/2}(I-B^2)^{1/2}\bigr)^2 = I - C^2,$$

and using [6, Lem. 3.11] we have

$$\bigl(I-C^2\bigr)^{1/2} = \bigl(-AB + (I-A^2)^{1/2}(I-B^2)^{1/2}\bigr)\mathrm{e}^{-\pi\mathrm{i}\,\mathcal{U}\left(2\log\left(-AB+(I-A^2)^{1/2}(I-B^2)^{1/2}\right)\right)}.$$

Since A and B have no eigenvalues in Ω, $\operatorname{asin} A$ and $\operatorname{asin} B$ both have eigenvalues with real parts in the interval $(-\frac{\pi}{2}, \frac{\pi}{2})$. Using the commutativity of A and B and Lemma 3.4 we then have $\mathcal{U}(\mathrm{i}\operatorname{asin} A + \mathrm{i}\operatorname{asin} B) = 0$. We can finally write

$$\operatorname{asin} A + \operatorname{asin} B = -\mathrm{i}\log\bigl(\mathrm{i}C + \bigl(I-C^2\bigr)^{1/2}\mathrm{e}^{\pi\mathrm{i}\,\mathcal{U}\left(2\log\left(-AB+(I-A^2)^{1/2}(I-B^2)^{1/2}\right)\right)}\bigr).$$

By Lemma 3.4 the unwinding term vanishes if and only if the arguments of all the eigenvalues of $-AB + (I-A^2)^{1/2}(I-B^2)^{1/2}$ lie in the interval $(-\pi/2, \pi/2]$. ∎

Now we give an analogous result for the inverse cosine.

THEOREM 3.9. *For all $A, B \in \mathbb{C}^{n\times n}$ with no eigenvalues in Ω and such that $AB = BA$,*

$$\operatorname{acos} A + \operatorname{acos} B = \operatorname{acos}\bigl(AB - (I-A^2)^{1/2}(I-B^2)^{1/2}\bigr) \tag{3.15}$$

if and only if the arguments of all the eigenvalues of $\mathrm{i}A(I-B^2)^{1/2}+\mathrm{i}B(I-A^2)^{1/2}$ *lie in the interval* $(-\pi/2,\pi/2]$ *and the real parts of the eigenvalues of* $\operatorname{acos}A+\operatorname{acos}B$ *lie in* $[0,\pi]$.

Proof. We omit the proof because it follows the same framework as the proof of Theorem 3.8. ∎

By definition, $\cos(\operatorname{acos}A)=A$, but the inverse relation $\operatorname{acos}(\cos A)=A$ does not always hold. In the next few theorems we give explicit formulas for $\operatorname{acos}(\cos A)$ and the counterparts for the sine and the inverse hyperbolic cosine and sine, and identify when these formulas reduce to A. These "round trip" formulas are new even in the scalar case. We note that scalar functional identities relating all four functions and their respective inverses are given in [14, App. B], but they have the unattractive feature that the identity for $\operatorname{acos}(\cos z)$ involves $\sin z$, and similarly for the other identities.

THEOREM 3.10. *If* $A\in\mathbb{C}^{n\times n}$ *has no eigenvalue with real part of the form* $k\pi$, $k\in\mathbb{Z}$, *then*

$$\operatorname{acos}(\cos A)=\big(A-2\pi\,\mathcal{U}(\mathrm{i}A)\big)\operatorname{sign}\big(A-2\pi\,\mathcal{U}(\mathrm{i}A)\big).$$

Proof. Let $B=A-2\pi\,\mathcal{U}(\mathrm{i}A)$. We first show that $\cos(B\operatorname{sign}B)=\cos A$. With $G=\operatorname{sign}B$ we have $\cos B=\cos(BG)$, which can be seen using the Jordan canonical form definitions of cos and sign along with the fact that $\cos(-X)=\cos X$ for any matrix X. Using the exponential representation (2.2) of the cosine function,

$$\begin{aligned}\cos B&=\frac{\mathrm{e}^{\mathrm{i}B}+\mathrm{e}^{-\mathrm{i}B}}{2}\\&=\frac{\mathrm{e}^{\mathrm{i}(A-2\pi\,\mathcal{U}(\mathrm{i}A))}+\mathrm{e}^{-\mathrm{i}(A-2\pi\,\mathcal{U}(\mathrm{i}A))}}{2}\\&=\frac{\mathrm{e}^{\mathrm{i}A}\mathrm{e}^{-2\pi\mathrm{i}\,\mathcal{U}(\mathrm{i}A)}+\mathrm{e}^{-\mathrm{i}A}\mathrm{e}^{2\pi\mathrm{i}\,\mathcal{U}(\mathrm{i}A)}}{2}.\end{aligned}$$

Now $\mathrm{e}^{2\pi\mathrm{i}\,\mathcal{U}(\mathrm{i}A)}=\mathrm{e}^{-2\pi\mathrm{i}\,\mathcal{U}(\mathrm{i}A)}=I$, since $\mathcal{U}(\mathrm{i}A)$ is diagonalizable and has integer eigenvalues [6, Lem. 3.5], so

$$\cos(BG)=\cos B=\frac{\mathrm{e}^{\mathrm{i}A}+\mathrm{e}^{-\mathrm{i}A}}{2}=\cos A.$$

Finally, since $\mathrm{i}B=\mathrm{i}A-2\pi\mathrm{i}\,\mathcal{U}(\mathrm{i}A)=\log\mathrm{e}^{\mathrm{i}A}$ by the definition (3.8) of the unwinding function, $\mathrm{i}B$ has eigenvalues with imaginary parts in the interval $(-\pi,\pi]$, hence B has eigenvalues with real parts in the interval $(-\pi,\pi]$. Therefore $B\operatorname{sign}B$ has eigenvalues with real parts in the interval $[0,\pi]$. We note that the end points of this interval are excluded because of the conditions in the statement of the theorem. Therefore the eigenvalues of B satisfy the condition in Definition 2.2 (a) (i). ∎

The following corollary of Theorem 3.10 gives necessary and sufficient conditions under which $A=\operatorname{acos}(\cos A)$ holds.

COROLLARY 3.11. *For* $A\in\mathbb{C}^{n\times n}$ *with no eigenvalue with real part of the form* $k\pi$, $k\in\mathbb{Z}$, $\operatorname{acos}(\cos A)=A$ *if and only if every eigenvalue of* A *has real part in the interval* $(0,\pi)$.

Proof. If all the eigenvalues of A satisfy the condition of this corollary, then, by Lemma 3.4, we have $\mathcal{U}(\mathrm{i}A)=0$. Then, since $\operatorname{sign}A=I$, by Theorem 3.10 we have $\operatorname{acos}(\cos A)=A$. Conversely, if $\operatorname{acos}(\cos A)=A$ then, since the condition of the corollary rules out A having an eigenvalue with real part 0 or π, the eigenvalues of A have real parts in the interval $(0, \pi)$, by Definition 2.2 (a). $\square$

THEOREM 3.12. *If $A \in \mathbb{C}^{n\times n}$ has no eigenvalue with real part of the form $(2k+1)\pi/2$, $k \in \mathbb{Z}$, then*

$$\operatorname{asin}(\sin A) = \mathrm{e}^{\pi \mathrm{i}\,\mathcal{U}(2\mathrm{i}A)}\big(A - \pi\,\mathcal{U}(2\mathrm{i}A)\big).$$

Proof. Let $C = A - \pi\,\mathcal{U}(2\mathrm{i}A)$ and $H = \mathrm{e}^{\pi\mathrm{i}\,\mathcal{U}(2\mathrm{i}A)}$. We will first prove that $\sin(HC) = \sin A$.

The matrix unwinding function $\mathcal{U}(2\mathrm{i}A)$ is diagonalizable with integer eigenvalues, so the matrix H is diagonalizable with eigenvalues equal to ± 1. It is not hard to show that $\sin(HC) = H \sin C$. Now

$$\sin C = \sin\big(A - \pi\,\mathcal{U}(2\mathrm{i}A)\big) = \sin A \cos\big(\pi\,\mathcal{U}(2\mathrm{i}A)\big) - \cos A \sin\big(\pi\,\mathcal{U}(2\mathrm{i}A)\big).$$

Since $\mathcal{U}(2\mathrm{i}A)$ is diagonalizable and has integer eigenvalues, $\sin(\pi\,\mathcal{U}(2\mathrm{i}A)) = 0$. From the properties of H described above, $H = \mathrm{e}^{\pi\mathrm{i}\,\mathcal{U}(2\mathrm{i}A)} = \mathrm{e}^{-\pi\mathrm{i}\,\mathcal{U}(2\mathrm{i}A)}$, and so

$$\cos(\pi\,\mathcal{U}(2\mathrm{i}A)) = \frac{\mathrm{e}^{\pi\mathrm{i}\,\mathcal{U}(2\mathrm{i}A)} + \mathrm{e}^{-\pi\mathrm{i}\,\mathcal{U}(2\mathrm{i}A)}}{2} = H.$$

Therefore $\sin(HC) = H \sin C = H^2 \sin A = \sin A$, which completes the first part of the proof.

Finally, we show that every eigenvalue of HC satisfies the condition in Definition 2.2 (b). We note that the real parts of the eigenvalues of HC lie in $[-\pi, 2/\pi/2]$ and the conditions in the statement of the theorem exclude the end points of this interval, so conditions (ii) and (iii) in Definition 2.2 (b) need not be checked. Using the definition (3.8) of the unwinding function we have

$$\mathrm{i}C = \mathrm{i}A - \pi\mathrm{i}\,\mathcal{U}(2\mathrm{i}A) = \mathrm{i}A - \pi\mathrm{i}\left(\frac{2\mathrm{i}A - \log \mathrm{e}^{2\mathrm{i}A}}{2\pi\mathrm{i}}\right) = \frac{\log \mathrm{e}^{2\mathrm{i}A}}{2}.$$

Here log is the principal matrix logarithm, so C has eigenvalues with real parts in the interval $(-\pi/2, \pi/2]$, and therefore HC has eigenvalues with real parts in the interval $[-\pi/2, \pi/2]$. But, as already noted, the end points of this interval are excluded because of the assumptions in the statement of the theorem. $\square$

COROLLARY 3.13. *For $A \in \mathbb{C}^{n\times n}$ with no eigenvalue with real part of the form $(2k+1)/2\pi$, $k \in \mathbb{Z}$,* $\operatorname{asin}(\sin A) = A$ *if and only if every eigenvalue of A has real part in the interval* $(-\pi/2, \pi/2)$.

Proof. If the eigenvalues of A have real parts in the interval $(-\pi/2, \pi/2)$ then by Lemma 3.4 we have $\mathcal{U}(2\mathrm{i}A) = 0$. Applying Theorem 3.12 we then have $\operatorname{asin}(\sin A) = A$.

Conversely, if $\operatorname{asin}(\sin A) = A$ then, since the condition of the corollary rules out A having an eigenvalue with real part $\pm\pi/2$, the eigenvalues of A have real parts in the interval $(-\pi/2, \pi/2)$, by Definition 2.2 (b). $\square$

Similar results hold for the inverse hyperbolic cosine and sine functions.

THEOREM 3.14. *For $A \in \mathbb{C}^{n\times n}$ with no eigenvalue with imaginary part of the form $k\pi$, with odd $k \in \mathbb{Z}$, and no pure imaginary eigenvalue,*

$$\operatorname{acosh}(\cosh A) = \big(A - 2\pi\mathrm{i}\,\mathcal{U}(A)\big)\operatorname{sign}\big(A - 2\pi\mathrm{i}\,\mathcal{U}(A)\big).$$

Proof. Let $B = A - 2\pi\mathrm{i}\,\mathcal{U}(A)$. We follow the same framework as that in the proofs of the previous two results. First, we note that $\cosh(B \operatorname{sign} B) = \cosh B$. Expressing cosh in terms of exponentials we have

$$\begin{aligned}\cosh B &= \frac{1}{2}\big(\mathrm{e}^{A-2\pi\mathrm{i}\,\mathcal{U}(A)} + \mathrm{e}^{-A+2\pi\mathrm{i}\,\mathcal{U}(A)}\big)\\ &= \frac{1}{2}\big(\mathrm{e}^{A} + \mathrm{e}^{-A}\big) = \cosh A,\end{aligned}$$

where we used $\mathrm{e}^{\pm 2\pi\mathrm{i}\,\mathcal{U}(A)} = I$ [6, Lem. 3.5].

Finally, we have to show that the eigenvalues of $B \operatorname{sign} B$ satisfy the requirements of Definition 2.2 (c). Using the definition of the unwinding function, $B = A - 2\pi\mathrm{i}\,\mathcal{U}(A) = \log \mathrm{e}^{A}$, we see that the imaginary parts of the eigenvalues of B lie in $(-\pi, \pi]$. Therefore each eigenvalue of $B \operatorname{sign} B$ has eigenvalues with nonnegative real part and imaginary part in the interval $[-\pi, \pi]$. The end points of this interval and the case when the eigenvalues of $B \operatorname{sign} B$ are pure imaginary are excluded because of the assumptions in the statement of the theorem. Therefore the conditions of Definition 2.2 (c) are satisfied. ∎

COROLLARY 3.15. *For $A \in \mathbb{C}^{n\times n}$ with no eigenvalue with imaginary part of the form $k\pi$, for odd $k \in \mathbb{Z}$, and no pure imaginary eigenvalue,* $\operatorname{acosh}(\cosh A) = A$ *if and only if every eigenvalue of A has imaginary part in the interval $(-\pi, \pi)$ and positive real part.*

Proof. If the eigenvalues of A all have imaginary parts in the interval $(-\pi, \pi)$ then $\mathcal{U}(A) = 0$, and if they all have positive real parts then $\operatorname{sign} A = I$. Therefore Theorem 3.14 gives $\operatorname{acosh}(\cosh A) = A$. Conversely, if $\operatorname{acosh}(\cosh A) = A$ and if A satisfies the conditions of the corollary then the eigenvalues of A have imaginary parts in the interval $(-\pi, \pi)$ and positive real parts, by Definition 2.2 (c) (i). ∎

THEOREM 3.16. *If $A \in \mathbb{C}^{n\times n}$ has no eigenvalue with imaginary part of the form $(2k+1)\pi\mathrm{i}/2$, $k \in \mathbb{Z}$, then*

$$\operatorname{asinh}(\sinh A) = \mathrm{e}^{\pi\mathrm{i}\,\mathcal{U}(2A)}\big(A - \pi\mathrm{i}\,\mathcal{U}(2A)\big).$$

Proof. Suppose first that A does not have any eigenvalues whose imaginary parts are of the form $(2k+1)\pi/2, k \in \mathbb{Z}$. This implies that $\sin(-\mathrm{i}A)$ has no eigenvalues ± 1, so we can use the identity $\sinh A = \mathrm{i}\sin(-\mathrm{i}A)$ from (2.4) and Theorems 3.3 and 3.12 to write

$$\begin{aligned}\operatorname{asinh}(\sinh A) &= \operatorname{asinh}\big(\mathrm{i}\sin(-\mathrm{i}A)\big)\\ &= \mathrm{i}\operatorname{asin}\big(\sin(-\mathrm{i}A)\big)\\ &= \mathrm{i}\mathrm{e}^{\pi\mathrm{i}\,\mathcal{U}(2A)}\big(-\mathrm{i}A - \pi\,\mathcal{U}(2A)\big)\\ &= \mathrm{e}^{\pi\mathrm{i}\,\mathcal{U}(2A)}\big(A - \pi\mathrm{i}\,\mathcal{U}(2A)\big).\end{aligned}$$ ∎

COROLLARY 3.17. *For $A \in \mathbb{C}^{n\times n}$ with no eigenvalue with imaginary part of the form $(2k+1)\pi\mathrm{i}/2$, $k \in \mathbb{Z}$,* $\operatorname{asinh}(\sinh A) = A$ *if and only if every eigenvalue of A has imaginary part in the interval $(-\pi/2, \pi/2)$.*

Proof. If every eigenvalue of A has imaginary part in $(-\pi/2, \pi/2)$ then by Lemma 3.4 we have $\mathcal{U}(2A) = 0$ and Theorem 3.16 gives $\operatorname{asinh}(\sinh A) = A$.

Conversely, if $\operatorname{asinh}(\sinh A) = A$, by Definition 2.2 (d), since (d) (ii) and (d) (iii) are excluded by the assumptions on A, the eigenvalues of A must have imaginary parts in the interval $(-\pi/2, \pi/2)$. ∎

4. Conditioning. The absolute condition number of a function f at the matrix A is given by [21, sect. 3.1]

$$\mathrm{cond}_{\mathrm{abs}}(f, A) = \max_{E \neq 0} \frac{\|L_f(A, E)\|}{\|E\|}. \tag{4.1}$$

Here, L_f is the Fréchet derivative of f, which is a linear operator such that $f(A+E) = f(A) + L_f(A, E) + o(\|E\|)$.

To study the conditioning of the inverse sine and cosine we need only study one of them, in view of the relation given in the next result between the respective Fréchet derivatives.

Lemma 4.1. *For $A \in \mathbb{C}^{n\times n}$ with no eigenvalues in Ω in* (2.5)*,*

$$L_{\mathrm{acos}}(A, E) + L_{\mathrm{asin}}(A, E) = 0.$$

Proof. Fréchet differentiate (3.5). □

A simple relation also exists between the Fréchet derivatives of asin and asinh.

Lemma 4.2. *For $A \in \mathbb{C}^{n\times n}$ with no eigenvalues in Ω in* (2.5)*,*

$$L_{\mathrm{asin}}(A, E) = L_{\mathrm{asinh}}(\mathrm{i}A, E).$$

Proof. Fréchet differentiate (3.7) using the chain rule [21, Thm. 3.4]. □

We now study further the Fréchet derivative of acos. Assume that A has no eigenvalues in Ω. By [21, Thm. 3.5] we have

$$L_{\cos}\left(\mathrm{acos}\, A, L_{\mathrm{acos}}(A, E)\right) = E. \tag{4.2}$$

Recall the integral representation of the Fréchet derivative of the matrix cosine function [21, sect. 12.2]

$$L_{\cos}(A, E) = -\int_0^1 \left[\cos\left(A(1-t)\right) E \sin(At) + \sin\left(A(1-t)\right) E \cos(At)\right] \mathrm{d}t. \tag{4.3}$$

Substituting into the relation (4.2) we find that the Fréchet derivative of acos satisfies

$$\begin{aligned} E = -\int_0^1 &\left[\cos\left((1-t)\,\mathrm{acos}\, A\right) L_{\mathrm{acos}}(A, E) \sin\left(t\, \mathrm{acos}\, A\right)\right. \\ &\left. + \sin\left((1-t)\,\mathrm{acos}\, A\right) L_{\mathrm{acos}}(A, E) \cos\left(t\, \mathrm{acos}\, A\right)\right] \mathrm{d}t. \end{aligned} \tag{4.4}$$

If A and E commute then the relation (4.4) simplifies to $E = -L_{\mathrm{acos}}(A, E) \sin(\mathrm{acos}\, A)$. Now we can apply Lemma 3.7 to obtain the more useful expression

$$L_{\mathrm{acos}}(A, E) = -E(I - A^2)^{-1/2} \qquad (AE = EA). \tag{4.5}$$

Setting $E = I$ in (4.5) gives $L_{\mathrm{acos}}(A, I) = -(I - A^2)^{-1/2}$, and for any subordinate norm we obtain the bound

$$\mathrm{cond}_{\mathrm{abs}}(\mathrm{acos}, A) \geq \|(I - A^2)^{-1/2}\|.$$

The condition number is necessarily large when A has an eigenvalue close to 1 or -1, which are the branch points of acos.

One would also expect acos to be ill conditioned when a pair of eigenvalues lies close to, but on either side of, the branch cut. This is revealed by applying a general lower bound from [21, Thm. 3.14], which gives

$$\mathrm{cond}_{\mathrm{abs}}(\mathrm{acos}, A) \geq \max_{\lambda,\mu\in\Lambda(A)} |\,\mathrm{acos}[\mu,\lambda]|,$$

where $\Lambda(A)$ is the spectrum of A and the lower bound contains the divided difference $\mathrm{acos}[\lambda,\mu] = (\mathrm{acos}\,\lambda - \mathrm{acos}\,\mu)/(\lambda-\mu)$. For example, if $\lambda = -2+\varepsilon\mathrm{i}$ and $\mu = -2-\varepsilon\mathrm{i}$, with $0 < \varepsilon \ll 1$, then $\mathrm{acos}\,\lambda = \pi - \mathrm{acos}\,2 + O(\varepsilon)$ and $\mathrm{acos}\,\mu = \pi + \mathrm{acos}\,2 + O(\varepsilon)$, so $\mathrm{acos}[\lambda,\mu] = O(1/\varepsilon)$.

5. Algorithms.

Lemma 3.2 and Theorem 3.3 show that if we have an algorithm for computing any one of the four functions $\mathrm{acos}A$, $\mathrm{asin}A$, $\mathrm{acosh}A$, and $\mathrm{asinh}A$ then the others can be obtained from it, although this may necessitate using complex arithmetic for a real problem. In the next subsection we propose an algorithm for computing the principal matrix inverse cosine based on Padé approximation. In subsection 5.2 we consider an alternative algorithm for computing the inverse trigonometric and inverse hyperbolic functions via their logarithmic representations given in Theorem 3.1.

We exploit a Schur factorization $A = QTQ^*$, where Q is a unitary matrix and T is upper triangular with the eigenvalues of A on its diagonal, along with the property $f(A) = Qf(T)Q^*$. The problems of computing $\mathrm{acos}A$, $\mathrm{asin}A$, $\mathrm{acosh}A$, and $\mathrm{asinh}A$ are thus reduced to computing the same functions of the triangular matrix T. We will explain how Schur-free variants of the algorithms can also be constructed; these are of interest for situations in which a highly efficient implementation of the Schur decomposition is not available, as may be the case in certain parallel computing environments (for example, the Parallel Computing Toolbox in MATLAB 2016a does not have a function for the Schur decomposition).

5.1. Schur–Padé algorithm.

We develop an algorithm analogous to the inverse scaling and squaring method for computing the matrix logarithm.

For $\rho(A) < 1$, where ρ is the spectral radius, we can write $\mathrm{acos}A$ as the power series (in view of (3.5)) [32, eq. (4.24.1)]

$$\mathrm{acos}A = \frac{\pi}{2}I - \sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{4^k(2k+1)}A^{2k+1}, \quad \rho(A) < 1. \tag{5.1}$$

Alternatively, we can expand as a series in $I - A$ [32, eq. (4.24.2)]:

$$\mathrm{acos}A = 2^{1/2}(I-A)^{1/2}\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k(2k+1)}(I-A)^k, \quad \rho(I-A) < 2.$$

Here, to ensure the existence of $(I-A)^{1/2}$, we require that A have no eigenvalues equal to 1. Replacing A by $I - A$ gives, for nonsingular A,

$$\mathrm{acos}(I-A) = (2A)^{1/2}\sum_{k=0}^{\infty} \frac{\binom{2k}{k}}{8^k(2k+1)}A^k, \quad \rho(A) < 2. \tag{5.2}$$

We will employ Padé approximants of the function $f(x) = (2x)^{-1/2}\,\mathrm{acos}(1-x)$, which (5.2) shows is represented by a power series in x that converges for $|x| \leq 2$ and so should be well approximated by Padé approximants near the origin. Let

$r_m(x) = p_m(x)/q_m(x)$ denote the diagonal $[m/m]$ Padé approximant of $f(x)$, so that $p_m(x)$ and $q_m(x)$ are polynomials of degrees at most m.

We now consider the backward error of approximating acos. For $A \in \mathbb{C}^{n\times n}$ we define $h_m : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ by

$$(2A)^{1/2} r_m(A) = \operatorname{acos}\big(I - A + h_m(A)\big),$$

assuming that all of the eigenvalues of $(2A)^{1/2} r_m(A)$ have real parts in the interval $(0, \pi)$. We can rewrite this equation as

$$h_m(A) = \cos\big((2A)^{1/2} r_m(A)\big) - (I - A).$$

The relative backward error in approximating $\operatorname{acos}(I - A)$ by $(2A)^{1/2} r_m(A)$ is given by $\|h_m(A)\|/\|A\|$, and we wish to bound it by the unit roundoff for IEEE double precision arithmetic, $u = 2^{-53} \approx 1.11 \times 10^{-16}$; that is, we would like to ensure that

$$\frac{\|h_m(A)\|}{\|A\|} = \frac{\|\cos\big((2A)^{1/2} r_m(A)\big) - (I - A)\|}{\|A\|} \le u. \tag{5.3}$$

We now follow the same framework as for backward error analysis of the exponential [2] and the cosine and sine [5, sect. 2]. We have $r_m(x) = (2x)^{-1/2} \operatorname{acos}(1-x) + O(x^{2m+1})$, and so $h_m(x) = \cos((2x)^{1/2} r_m(x)) - (1 - x) = O(x^{2m+2})$, where the last equality is obtained after some manipulations.

We can write

$$h_m(A) = \sum_{\ell=0}^{\infty} c_\ell A^{2m+\ell+2} = A \sum_{\ell=0}^{\infty} c_\ell A^{2m+\ell+1}$$

for some coefficients c_ℓ. We now use [2, Thm. 4.2(a)] to obtain the bound on the relative backward error

$$\frac{\|h_m(A)\|}{\|A\|} \le \sum_{\ell=0}^{\infty} |c_\ell| \alpha_p(A)^{2m+\ell+1},$$

where

$$\alpha_p(A) = \max\big(\|A^p\|^{1/p}, \|A^{p+1}\|^{1/(p+1)}\big)$$

and p is an integer such that $2m + 1 \ge p(p - 1)$. It can be shown that $\alpha_1(A) \ge \alpha_2(A) \ge \alpha_3(A)$, but for $p \ge 4$ the relation between $\alpha_{p-1}(A)$ and $\alpha_p(A)$ depends on the matrix A. We need to find the smallest value of $\alpha_p(A)$ subject to the constraint $2m + 1 \ge p(p - 1)$.

With the definition

$$\beta_m = \max\left\{\beta : \sum_{\ell=0}^{\infty} |c_\ell| \beta^{2m+\ell+1} \le u\right\},$$

the inequality $\alpha_p(A) \le \beta_m$ implies that the relative backward error is bounded by u. Table 5.1 gives the values of β_m for a range of values of m, determined experimentally using a combination of high precision arithmetic and symbolic calculations, in a similar way as in [22].

Table 5.1 also gives the number of matrix multiplications π_m required to evaluate the Padé approximant $r_m(A)$ of order $[m/m]$ using the Paterson–Stockmeyer scheme [21, sect. 4.2 and Table 4.2], [33] for both p_m and q_m.

TABLE 5.1
Values of β_m, values of p to be considered, and number of matrix multiplications π_m required to evaluate r_m.

m	1	2	3	4	5	6
β_m	3.44e-5	4.81e-3	3.97e-2	1.26e-1	2.59e-1	4.17e-1
$p \le$	2	2	3	3	3	4
π_m	0	1	2	3	4	4

m	7	8	9	10	11	12
β_m	5.81e-1	7.39e-1	8.84e-1	1.01	1.13	1.22
$p \le$	4	4	4	5	5	5
π_m	5	5	6	6	7	7

To ensure that $\alpha_p(A) \le \beta_m$ for a suitable value of m we use repeatedly the identity $\operatorname{acos} X = 2 \operatorname{acos}\big(((I+X)/2)^{1/2}\big)$ in (3.11), which brings the argument close to the identity, as shown by the next result.

LEMMA 5.1. *For any $X_0 \in \mathbb{C}^{n\times n}$, the sequence defined by*

$$X_{k+1} = \left(\frac{I+X_k}{2}\right)^{1/2} \tag{5.4}$$

satisfies $\lim_{k\to\infty} X_k = I$.

Proof. First, consider the scalar iteration $x_{k+1} = ((1+x_k)/2)^{1/2}$. It is easy to see that

$$x_{k+1} - 1 = \frac{x_k - 1}{2\left(\left(\frac{1+x_k}{2}\right)^{1/2} + 1\right)}$$

and hence that $|x_{k+1} - 1| \le |x_k - 1|/2$, since $\operatorname{Re}((1+x_k)/2)^{1/2} \ge 0$. Therefore $\lim_{k\to\infty} x_k = 1$. The function $((1+x)/2)^{1/2}$ is holomorphic for $\operatorname{Re} x \ge 0$, and furthermore its derivative at $x = 1$ satisfies $|\frac{d}{dx}(\frac{1}{2}(x+1)^{1/2}|_{x=1} = \frac{1}{4} < 1$. The convergence of the matrix iteration follows from a general result of Iannazzo [26, Thm. 3.20]. ☐

We apply the recurrence (5.4) with $X_0 = T$, selecting the scaling parameter s so that $\alpha_p(I - X_s) \le \beta_m$. To compute the square roots required to obtain X_s we use the Björck–Hammarling method [8], [21, Alg. 6.3]. Increasing the scaling parameter s by 1 has a cost of $n^3/3$ flops, so it is worth doing if it decreases the number of (triangular) matrix multiplications, which also cost $n^3/3$ flops each, by more than 1. From the relation

$$(I - X_{s+1})(I + X_{s+1}) = I - X_{s+1}^2 = I - \frac{I+X_s}{2} = \frac{I - X_s}{2}, \tag{5.5}$$

it is clear that for large s (so that $X_s \approx I$), $\alpha_p(I - X_{s+1}) \approx \alpha_p(I - X_s)/4$. From the values of β_m in Table 5.1 we see that for $m \ge 9$ it is more efficient to continue the recursion and consequently use an approximant of a lower degree. Indeed for $m = 9$, $\beta_9/4 = 2.21\text{e-}1 < 2.59\text{e-}1 = \beta_5$, so the effect of taking an extra step in the recursion would be that we could use an approximant of type [5/5], and so the number of matrix multiplications required would be reduced from 6 to 4.

In computing $\alpha_p(A)$ we avoid explicit computation of powers of A by estimating $\|A^p\|_1^{1/p}$ and $\|A^{p+1}\|_1^{1/(p+1)}$ using the block 1-norm estimator of Higham and Tisseur [24].

A further computational saving can be provided by computing a lower bound on the scaling parameter s. Denote by $D = \operatorname{diag}(T)$ the diagonal matrix containing the eigenvalues of A on its diagonal and observe that $\rho(I - D) = \rho(I - T) \le \alpha_p(I - T)$. The largest β we consider is β_8, and the inequality $\alpha_p(I - T) \le \beta_8$ also requires that $\rho(I - D) \le \beta_8$, so we can apply the recurrence (5.4) to the matrix D to obtain a lower bound s_0 on s at negligible cost.

We are now ready to state the algorithm for computing acos. In the pseudocode the statement "break" denotes that execution jumps to the first statement after the while loop.

ALGORITHM 5.2 (Schur–Padé algorithm). *Given $A \in \mathbb{C}^{n\times n}$ with no eigenvalues equal to ± 1, this algorithm computes $X = \operatorname{acos} A$. The algorithm is intended for use with IEEE double precision arithmetic.*

Compute the Schur decomposition $A = QTQ^*$ (Q unitary, T upper triangular).
Find s_0, the smallest s such that $\rho(I - X_s) \le \beta_8$, where the X_s are the iterates from (5.4) with $X_0 = \operatorname{diag}(T)$.
for $i = 1\colon s_0$
  $T = \left(\frac{1}{2}(I + T)\right)^{1/2}$
end
$s = s_0$, $m = 0$
while $m = 0$
  $Z = I - T$
  Estimate $d_2(Z) = \|Z^2\|_1^{1/2}$.
  Estimate $d_3(Z) = \|Z^3\|_1^{1/3}$.
  $\alpha_2(Z) = \max(d_2, d_3)$
  if $\alpha_2(Z) \le \beta_1$, $m = 1$, break, end
  if $\alpha_2(Z) \le \beta_2$, $m = 2$, break, end
  Estimate $d_4(Z) = \|Z^4\|_1^{1/4}$.
  $\alpha_3(Z) = \max(d_3, d_4)$
  if $\alpha_3(Z) \le \beta_3$, $m = 3$, break, end
  if $\alpha_3(Z) \le \beta_4$, $m = 4$, break, end
  if $\alpha_3(Z) \le \beta_5$, $m = 5$, break, end
  Estimate $d_5(Z) = \|Z^5\|_1^{1/5}$.
  $\alpha_4(Z) = \max(d_4, d_5)$
  $\gamma(Z) = \min(\alpha_3(Z), \alpha_4(Z))$
  if $\gamma(Z) \le \beta_6$, $m = 6$, break, end
  if $\gamma(Z) \le \beta_7$, $m = 7$, break, end
  if $\gamma(Z) \le \beta_8$, $m = 8$, break, end
  $T = \left(\frac{1}{2}(I + T)\right)^{1/2}$
  $s = s + 1$
end
Compute $U = r_m(Z)$ by using the Paterson–Stockmeyer scheme to evaluate $p_m(Z)$ and $q_m(Z)$ and then solving $q_m(Z)U = p_m(Z)$.
$Y = Z^{1/2}$
$V = 2^{1/2}UY$
$W = 2^s V$
$X = QWQ^*$

Cost: $25n^3$ flops for the Schur decomposition, $sn^3/3$ flops to compute the square roots for the scaling stage, $(\pi_m + 1)n^3/3$ flops to compute the Padé approximation of order $[m/m]$, $n^3/3$ flops for the final square root, and $3n^3$ flops to form X: about $(28\frac{2}{3} + \frac{\pi_m+s}{3})n^3$ flops in total.

Note that Algorithm 5.2 requires only that A have no eigenvalues on the branch points of acos; eigenvalues may lie anywhere else on the branch cuts.

A Schur-free variant of Algorithm 5.2 can be obtained by removing lines 1–5 and 32, setting $s = 0$ on line 6, and computing the square roots using (for example) a scaled Denman–Beavers iteration [21, sect. 6.3].

The other functions of interest can be computed by using Algorithm 5.2 in conjunction with the formulas, from Lemma 3.2 and Theorem 3.3,

$$\operatorname{asin} A = (\pi/2)I - \operatorname{acos} A, \tag{5.6}$$

$$\operatorname{asinh} A = \mathrm{i}\,\operatorname{asin}(-\mathrm{i}A) = \mathrm{i}\big((\pi/2)I - \operatorname{acos}(-\mathrm{i}A)\big), \tag{5.7}$$

$$\operatorname{acosh} A = \mathrm{i}\,\operatorname{sign}(-\mathrm{i}A)\operatorname{acos} A \quad \text{if } A \text{ has no eigenvalues in } (0,1]. \tag{5.8}$$

The last relation requires computation of the matrix sign function of a triangular matrix (exploiting the Schur form), which can be done by [21, Alg. 5.5] at a cost of up to $2n^3/3$ flops, with a further $n^3/3$ flops for the final (triangular) matrix multiplication. A fast, blocked implementation of [21, Alg. 5.5] has recently been developed by Stotland, Schwartz, and Toledo [38]. The relation (5.6) may suffer from subtractive cancellation when $A \approx 0$; in this case we can simply take a few terms of the power series in (5.1); similarly for (5.7).

For a Schur-free algorithm, the matrix sign function can be computed using a Newton algorithm or some other rational iteration [21, Chap. 5], [31]. Equation (5.8) is applicable only when A has no eigenvalue in the interval $(0,1]$. When this condition is not satisfied acosh can be computed using the logarithmic representations of acosh given in (3.3), as described in the next subsection. Alternatively, a special purpose algorithm could be designed, using analysis similar to that in subsection 5.1.

5.2. Algorithms based on logarithmic formulas. Another way to compute the matrix inverse trigonometric and inverse hyperbolic functions is via their logarithmic representations given in Theorem 3.1. The most popular method for computing the matrix logarithm is the inverse scaling and squaring method. It was introduced by Kenney and Laub [28] and has undergone extensive development [3], [11], [13], [21, sect. 11.5], with special attention to computation in real arithmetic [4], [17]. The inverse scaling and squaring method is based on the relation $\log X = 2^s \log(X^{1/2^s})$ for $s \in \mathbb{Z}$, with s taken sufficiently large that $X^{1/2^s}$ is close to the identity matrix and a Padé approximant to $\log(1+x)$ used to approximate $\log(X^{1/2^s})$. In the most recent algorithms the degree of the Padé approximant is variable.

Using the first formula in (3.1) we obtain the following algorithm.

ALGORITHM 5.3. *Given $A \in \mathbb{C}^{n\times n}$ with no eigenvalues equal to ± 1, this algorithm computes $C = \operatorname{acos} A$ via the matrix logarithm.*

Compute the Schur decomposition $A = QTQ^*$.
$R = (I - T^2)^{1/2}$
Compute $X = -\mathrm{i}\log(T + \mathrm{i}R)$ using [3, Alg. 4.1].
$C = QXQ^*$

Cost: $25n^3$ flops for the Schur decomposition, $2n^3/3$ flops to compute R, $(\hat{s} + \hat{m})n^3/3$ flops to compute X (where $\hat{s}$ is the scaling parameter in the inverse scaling and squaring method and $\hat{m}$ is the degree of the Padé approximation used), plus $3n^3$ flops to form C: about $(28\frac{2}{3} + \frac{\hat{s}+\hat{m}}{3})n^3$ flops in total.

A Schur-free algorithm can be obtained by omitting the first and last lines of the algorithm, replacing T by A on lines 2–3, and computing the logarithm using [3, Alg. 5.2].

Corresponding algorithms for asin, acosh, and asinh are obtained by using (3.2), the first formula in (3.3), and (3.4).

In the `linear-algebra` package of GNU Octave (version 4.0.0) [18], the function `thfm.m` ("trigonometric/hyperbolic functions of square matrix") implements logarithmic formulas for acos, asin, acosh, and asinh. This function has two weaknesses. First, the formula used for acosh is $\operatorname{acosh} A = \log(A + (A^2 - I)^{1/2})$, which differs from (3.3) (cf. Lemma 3.5) and does not produce the principal branch as we have defined it. Second, the formulas are implemented as calls to `logm` and `sqrtm`, and so two Schur decompositions are computed rather than one.

6. Numerical experiments. We present numerical experiments with the following algorithms.

- Algorithm 5.2, which computes acos by the Schur–Padé algorithm. In the case of asin, acosh, and asinh, the algorithm is used together with (5.6)–(5.8). In (5.8) the sign function of a triangular matrix is computed with the function `signm` from [20]. When (5.8) is not applicable we use the first logarithmic formula for acosh in (3.3).
- Algorithm 5.3 and its counterparts for asin, acosh, and asinh based on the logarithmic representations.

We note that an algorithm for computing the matrix inverse hyperbolic sine has been proposed by Cardoso and Silva Leite [10, Alg. 1]. They compute $\operatorname{asinh} A$ using its logarithmic representation (3.4). In computing the logarithm they use the relation $\log((1+x)/(1-x)) = 2 \operatorname{atanh} x$, where atanh is the inverse hyperbolic tangent, along with Padé approximations of atanh. The degree of the Padé approximant is fixed at 8 and is not chosen optimally. For this reason we will not consider this algorithm further.

All computations are performed in MATLAB 2016a, for which the unit roundoff is $u \approx 1.11 \times 10^{-16}$.

We consider a set of 20 test matrices, which are mostly 10×10 and are based on matrices from the MATLAB `gallery` function, the Matrix Computation Toolbox [19], test problems provided with EigTool [39], and matrix exponential test problems [2]. We excluded all matrices that caused overflow or that had eigenvalues at the branch points of any of the four functions. Two of the matrices have an eigenvalue exactly on the branch cuts of some of the functions. Many of the test matrices have eigenvalues close to the branch cuts, where ill conditioning occurs. It is important to note that since the branch cuts are points of discontinuity one cannot expect an algorithm for these functions always to be accurate when an eigenvalue lies exactly on the branch cut, since a single rounding error in the Schur reduction can move the eigenvalue off the branch cut and produce a very large change in the function.

Figure 6.1 gives the relative errors $\| \operatorname{acos} A - \widehat{C} \|_1 / \| \operatorname{acos} A \|_1$. Here, an accurate $\operatorname{acos} A$ was obtained using 100-digit arithmetic with the Advanpix Multiprecision Computing Toolbox for MATLAB [30], exploiting the eigendecomposition $A = VDV^{-1}$ and the property $f(A) = Vf(D)V^{-1}$. For each matrix we also estimated the relative condition number

$$\operatorname{cond}_{\mathrm{rel}}(f, A) = \frac{\operatorname{cond}_{\mathrm{abs}}(f, A) \|A\|}{\|f(A)\|},$$

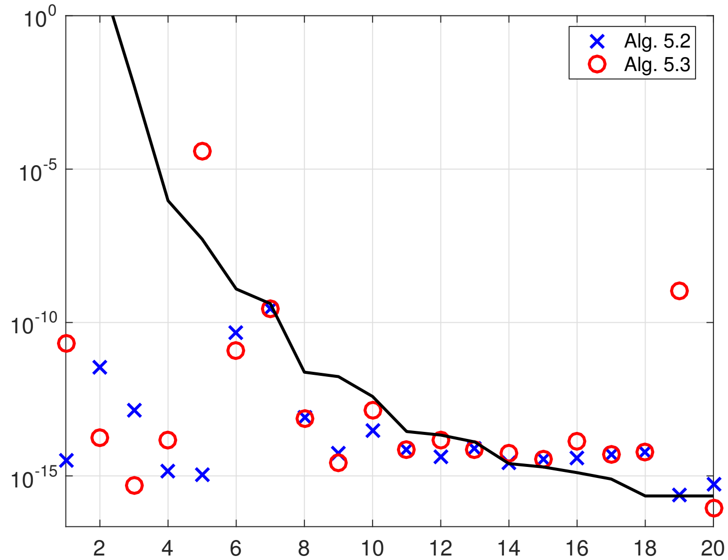

FIG. 6.1. *Relative error in computing* acos$A$ *using Algorithms* 5.2 *and* 5.3. *The solid line is* $\mathrm{cond}_{\mathrm{acos}}(A)u$.

where $\mathrm{cond}_{\mathrm{abs}}$ is defined in (4.1), using the algorithm `funm_condest1` from the Matrix Function Toolbox [20], which implements [21, Alg. 3.22]. The latter algorithm requires the Fréchet derivatives $L_{\mathrm{acos}}(A, E)$, which are obtained using the identity [21, Thm. 3.6], [29]

$$\mathrm{acos}\left(\begin{bmatrix} A & E \\ 0 & A \end{bmatrix}\right) = \begin{bmatrix} \mathrm{acos}\,A & L_{\mathrm{acos}}(A, E) \\ 0 & \mathrm{acos}\,A \end{bmatrix}, \tag{6.1}$$

and we use Algorithm 5.2 for this computation. We use Lemmas 4.1 and 4.2 to obtain the Fréchet derivatives of asin and asinh, and the analogue of (6.1) for acosh, along with (5.8), to obtain the Fréchet derivative of acosh.

Figures 6.2–6.4 give the 1-norm relative errors for asin, acosh, and sinh computed using the variants of Algorithm 5.3, based on the matrix logarithm.

For all four functions it can be seen that Algorithm 5.2 gives the best results overall and behaves in a forward stable fashion, that is, the relative error is not much larger than $\mathrm{cond}_{\mathrm{rel}}(f, A)u$. The algorithms based on the logarithmic representations have a major disadvantage. The branch point of the logarithm is at zero, and so when the argument of the logarithm has an eigenvalue close to this branch point there may be large relative errors in computing the logarithm. However, the argument of the logarithm can have eigenvalues close to zero when the argument of asin, acos, asinh, or acosh is not close to a branch point of that function. Consider, for example, a matrix A with some eigenvalues with large negative imaginary parts. The corresponding eigenvalues of $A + \mathrm{i}(I - A^2)^{1/2}$ are close to zero, which may be detrimental for the computation of the logarithm in Algorithm 5.3. We observed this for the matrix indexed 19 in Figure 6.1. A slightly modified version of this matrix is

$$A = \begin{bmatrix} 0 & b \\ -b & 0 \end{bmatrix}, \quad b = 1000,$$

with eigenvalues $\pm 1000\mathrm{i}$. The eigenvalues of $A + \mathrm{i}(I - A^2)^{1/2}$ are approximately $5 \times$

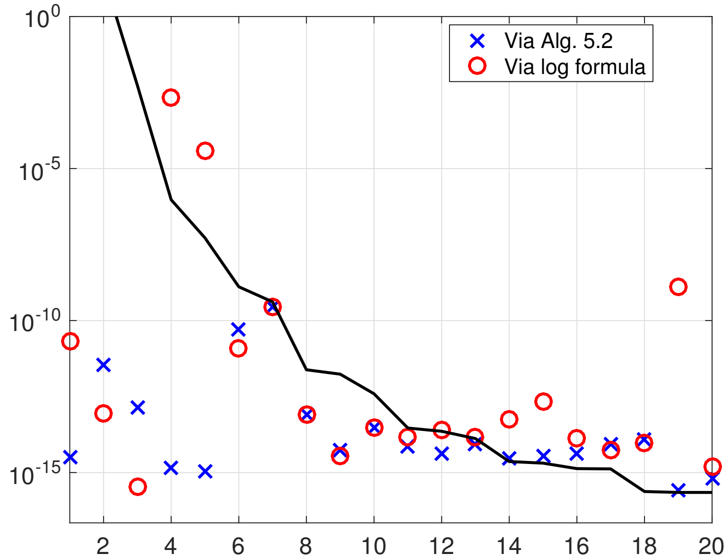

FIG. 6.2. *Relative error in computing* asin A *using Algorithm* 5.2 (*with* (5.6)) *and via log formula* (*variant of Algorithm* 5.3). *The solid line is* $\mathrm{cond}_{\mathrm{asin}}(A)u$.

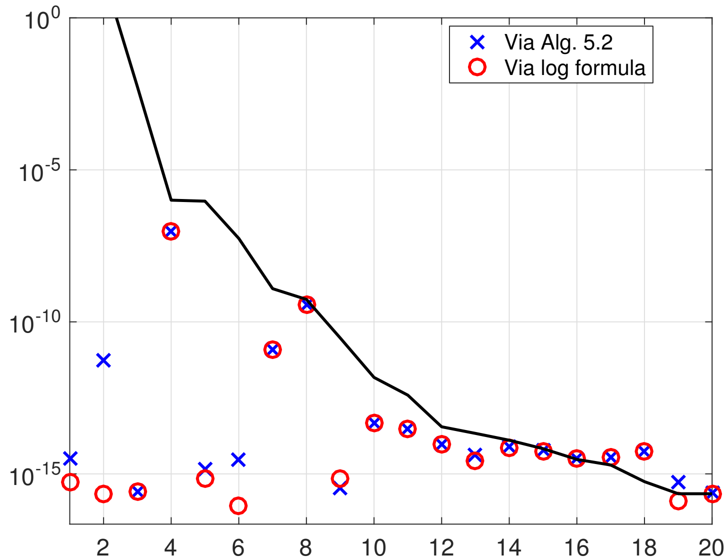

FIG. 6.3. *Relative error in computing* acosh A *using Algorithm* 5.2 (*with* (5.8)) *and via log formula* (*variant of Algorithm* 5.3). *The solid line is* $\mathrm{cond}_{\mathrm{acosh}}(A)u$.

10^{-4}i and 2000i, so one of them is very close to zero, and this is reflected in the relative error for Algorithm 5.3 for computing acos, which is $\|\operatorname{acos} A - \widehat{C}\|_1/\|\operatorname{acos} A\|_1 \approx 1.98 \times 10^{-9}$ versus 3.68×10^{-16} for Algorithm 5.2. This is not surprising in view of the large difference between the (estimated) relative 1-norm condition numbers, which are 0.83 for acos A and 2.1×10^7 for $\log(A + \mathrm{i}(I - A^2)^{1/2})$.

Finally, we reiterate that acosh A can be computed using Algorithm 5.2 and (5.8) only if A has no eigenvalue in the interval $(0, 1]$. This restriction was satisfied for all

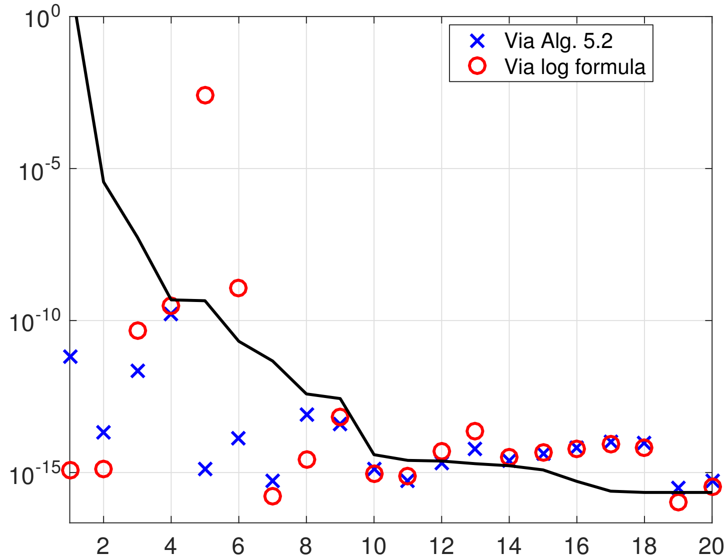

FIG. 6.4. *Relative error in computing* $\operatorname{asinh} A$ *using Algorithm* 5.2 (*with* (5.7)) *and via log formula* (*variant of Algorithm* 5.3). *The solid line is* $\operatorname{cond}_{\operatorname{asinh}}(A)u$.

but two of the matrices—those indexed 3 and 7 in Figure 6.3. However, as we see from the figure, the acosh variant of Algorithm 5.3 provides a good alternative for such cases.

7. Concluding remarks. The goals of this work were to study matrix inverse trigonometric and inverse hyperbolic functions and to derive algorithms for their computation. We characterized when the functions exist. We defined the principal matrix functions, asin, acos, asinh, and acosh, precisely specifying the values they attain on their respective branch cuts, and proved that they exist, are unique, and are primary matrix functions. We showed that many identities known to hold for real scalars can be extended to complex matrices. We also derived some identities that are new even in the scalar case, namely, a relation between $\operatorname{acosh} A$ and $\operatorname{acos} A$ (Theorem 3.3) and "round trip" identities that yield necessary and sufficient conditions for $\operatorname{acos}(\cos A)$ to equal A, and similarly for the other functions (Theorems 3.10, 3.12, 3.14, and 3.16). In addition, we obtained insight into the conditioning of the functions. Essential tools in our analyses are the matrix unwinding function and the matrix sign function. An important feature of all our results is that, unlike many treatments of their scalar counterparts, all choices of branches and signs are precisely specified.

Our new Schur–Padé algorithm for acos, Algorithm 5.2, performs in a forward stable fashion in our experiments and is clearly superior in accuracy to the algorithm based on the logarithm, which has the disadvantage of being susceptible to the sensitivity of the logarithm near the origin. Algorithm 5.2, combined with (5.6)–(5.8) for asin, acosh, and asinh, forms the first numerically reliable set of algorithms for computing these matrix functions.

Our MATLAB implementations of Algorithm 5.2, and the variants for asin, acosh, and asinh, can be found at https://github.com/higham/matrix-inv-trig-hyp.

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