Challenges in Multivalued Matrix Functions

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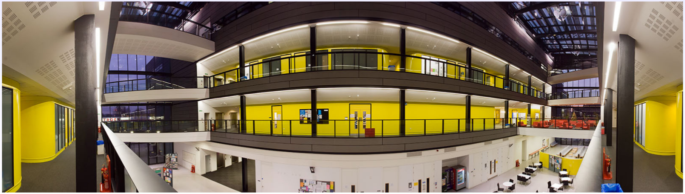

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Outline

1. The Trouble with Multivalued Functions
2. The Matrix Logarithm and Matrix Unwinding Function
3. Matrix Inverse Trigonometric & Hyperbolic Functions
4. Algorithms

Multivalued (Inverse) Functions

- log, acos, asin, acosh, asinh, . . .
- **Branch cuts** help define connected domain where f analytic.
- Location of branch cuts is otherwise arbitrary.
- Define **principal values** (distinguished branches), including values on the branch cuts.

Issues for Numerical Computation

- Branch cuts and choices of branch must be consistent between different inverse functions.
- Choices must be clearly documented.
- Precisely when do identities hold?

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For matrices:

- Existence.
- Uniqueness of principal values.
- Validity of identities: more than just the scalar case.
- Computation.

Quotes (1)

Corless et al. (2000):

Definitions of the elementary functions are given in many textbooks and mathematical tables . . .
often require a great deal of common sense to interpret them, or . . .
are **blatantly self-inconsistent**

Quotes (2)

Penfield (1981):

One cannot find in the mathematics or computer-science literature a **definitive value for** the principal value of the arcsin of 3.

Kahan (1987):

Principal Values have too often been left **ambiguous on the slits**, causing **confusion and controversy** . . .

Comparing various definitions, and choosing among them, is a **tedious business prone to error**.

The Scalar Logarithm: Comm. ACM

- J. R. Herndon (1961). **Algorithm 48: Logarithm of a complex number**.

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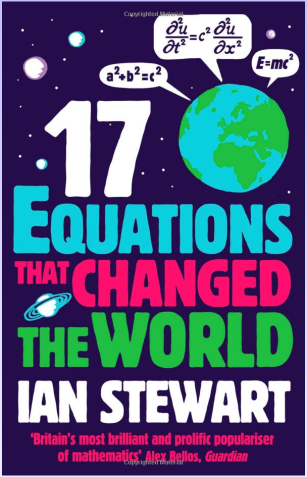
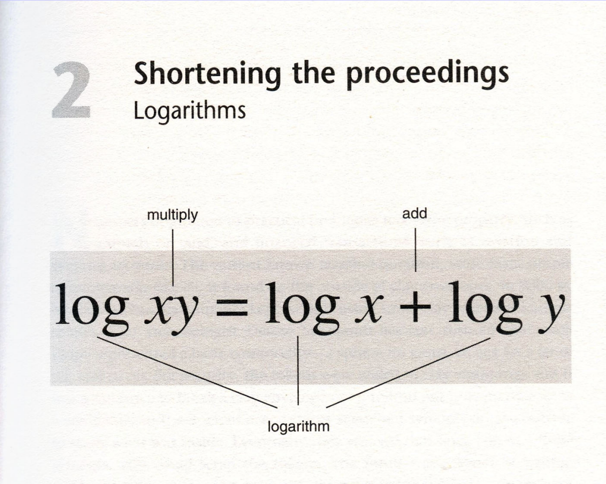
- D. S. Collens (1964). **Algorithm 243: Logarithm of a complex number: Rewrite of Algorithm 48.**





One of my choices for **Five Books**.

Logarithm of Product, Complex Case

$$\text{(iii)}.\ \log z_1 z_2 = \log z_1 + \log z_2 \tag{9.1}$$

$$\log\left(\frac{z_1}{z_2}\right) = \log z_1 - \log z_2. \tag{9.2}$$

Indeed, we have

$$\begin{aligned}
\log z_1 z_2 &= \operatorname{Log}|z_1 z_2| + i \arg z_1 z_2 \\
&= \operatorname{Log}|z_1| + \operatorname{Log}|z_2| + i \arg z_1 + i \arg z_2 \\
&= \log z_1 + \log z_2.
\end{aligned}$$

R.P. Agarwal et al., *An Introduction to Complex Analysis*, 57

DOI 10.1007/978-1-4614-0195-7_9,

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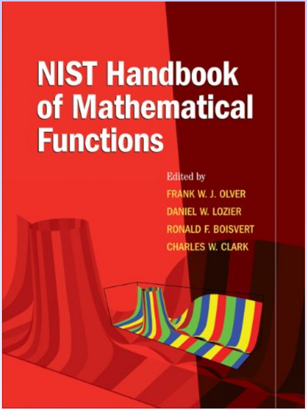
Goes on to say must take appropriate branch for each occurrence of log.

NIST Handbook (Olver et al. 2010)



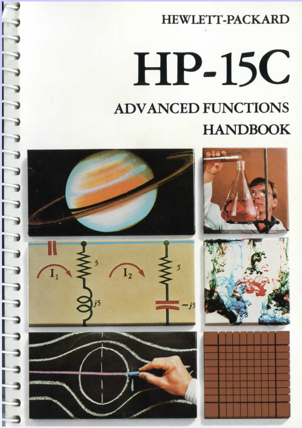
4.24(iii) Addition Formulas

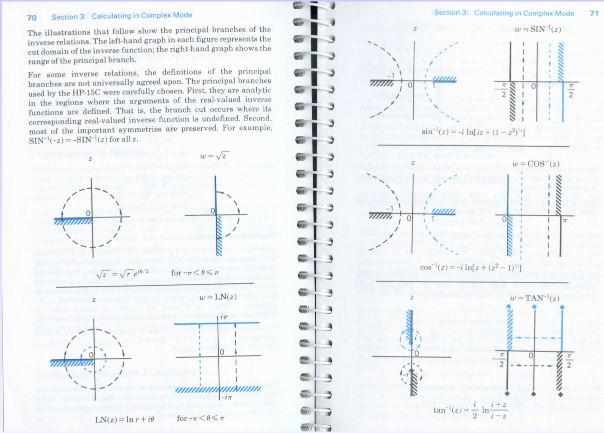
4.24.13
$$\operatorname{Arcsin} u \pm \operatorname{Arcsin} v = \operatorname{Arcsin}\left(u(1-v^2)^{1/2} \pm v(1-u^2)^{1/2}\right),$$

4.24.14
$$\operatorname{Arccos} u \pm \operatorname{Arccos} v = \operatorname{Arccos}\left(uv \mp ((1-u^2)(1-v^2))^{1/2}\right),$$

Arcsin, Arccos are “general values” of inverse sine, inverse cosine.

HP-15C Handbook (1982 and 1986)

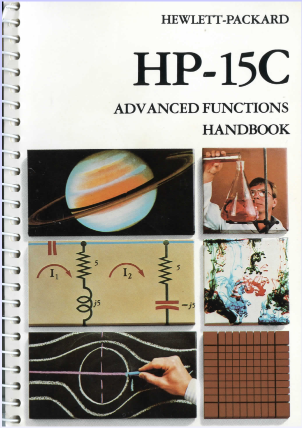


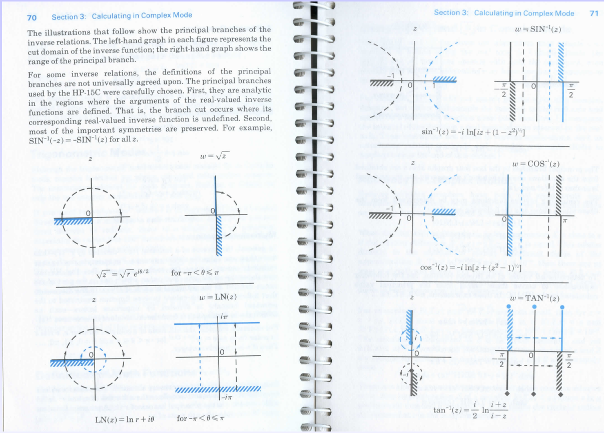


The illustrations that follow show the principal branches of the inverse relations. The left-hand graph in each figure represents the cut domain of the inverse function; the right-hand graph shows the range of the principal branch.

For some inverse relations, the definitions of the principal branches are not universally agreed upon. The principal branches used by the HP-15C were carefully chosen. First, they are analytic in the regions where the arguments of the real-valued inverse functions are defined. That is, the branch cut occurs where its corresponding real-valued inverse function is undefined. Second, most of the important symmetries are preserved. For example, $\mathrm{SIN}^{-1}(-z) = -\mathrm{SIN}^{-1}(z)$ for all z.

HP-15C Handbook (1982 and 1986)





acos formula "quite wrong" (Kahan, 1987)

MATLAB and Symbolic Math Toolbox

```
>> z = -4; acosh(z), double(acosh(sym(z)))
ans =
   2.0634e+00 + 3.1416e+00i
ans =
  -2.0634e+00 + 3.1416e+00i
```

Identities in Complex Variables

$$(1-z)^{1/2}(1+z)^{1/2} = (1-z^2)^{1/2} \quad \text{for all } z,$$

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$$(z-1)^{1/2}(z+1)^{1/2} = (z^2-1)^{1/2} \quad \text{for } \boxed{\arg z \in (-\pi/2, \pi/2]}.$$

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$$(z-1)^{1/2}(z+1)^{1/2} = (z^2-1)^{1/2} \quad \text{for } \boxed{\arg z \in (-\pi/2, \pi/2]}.$$

Need to be very careful in simplifying expressions involving multivalued functions.

- When is $\log e^z = z$?
- When is $\operatorname{acos}(\cos z) = z$?

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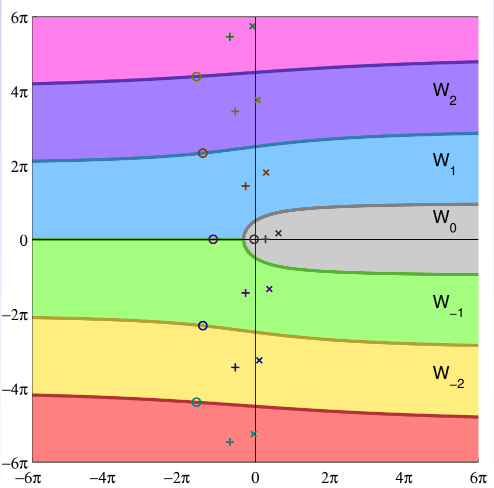
Logarithm and Square Root

- X is a logarithm of $A \in \mathbb{C}^{n\times n}$ if $e^X = A$. Write $X = \log A$.
- Branch cut $(-\infty, 0]$.
- **Principal logarithm**, $\log A$: $\operatorname{Im} \lambda(\log A) \in (-\pi, \pi]$.
- **Principal square root**: $X^2 = A$ and $\operatorname{Re} \lambda(X) \geq 0$, $(-r)^{1/2} = r^{1/2} i$ for $r \geq 0$.

The Lambert W Function

$W_k(a)$, $k \in \mathbb{Z}$: solutions of $we^w = a$.



Fasi, H & Iannazzo: *An Algorithm for the Matrix Lambert W Function*, SIMAX (2015).

Unwinding Number

Definition

$$\mathcal{U}(z) = \frac{z - \log e^z}{2\pi i}.$$

Note:

$$z = \log e^z + 2\pi i\,\mathcal{U}(z).$$

- Corless, Hare & Jeffrey (1996);
- Apostol (1974): special case.

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ISO standard typesetting!

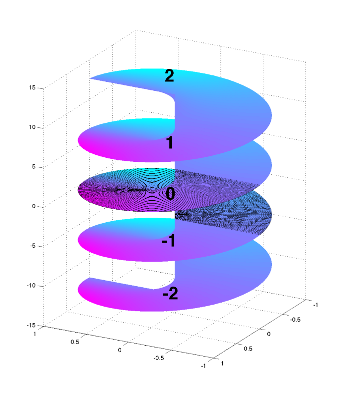
Unwinding number is an integer

$$\mathcal{U}(z) = \frac{z - \log e^z}{2\pi i} = \left\lceil \frac{\operatorname{Im} z - \pi}{2\pi} \right\rceil .$$

When is $\log(e^z) = z$?

$\mathcal{U}(z) = 0$ iff $\operatorname{Im} z \in (-\pi, \pi]$.

Riemann surface of logarithm



Matrix Unwinding Function

H & Aprahamian (2014):

$$\boxed{\mathcal{U}(A) = \frac{A - \log e^A}{2\pi i},} \qquad A \in \mathbb{C}^{n\times n}.$$

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Jordan form

For $Z^{-1}AZ = \mathrm{diag}(J_k(\lambda_k))$,

$$U(A) = Z\mathrm{diag}(U(\lambda_k)I_{m_k})Z^{-1}.$$

- $U(A)$ is diagonalizable.
- $U(A)$ has integer ei'vals.
- $U(A)$ is pure imaginary if A is real.

Logarithm of Matrix Product

Theorem (Aprahamian & H, 2014)

Let $A, B \in \mathbb{C}^{n\times n}$ be nonsingular and $AB = BA$. Then

$$\log(AB) = \log A + \log B - 2\pi \mathrm{i}\,\mathcal{U}(\log A + \log B).$$

Power of a Product

Theorem

Let $A, B \in \mathbb{C}^{n\times n}$ be nonsingular and $AB = BA$. For $\alpha \in \mathbb{C}$,

$$(AB)^\alpha = A^\alpha B^\alpha \mathrm{e}^{-2\pi\alpha \mathrm{i}\,\mathcal{U}(\log A + \log B)}.$$

Proof.

$$\begin{aligned}(AB)^\alpha &= \mathrm{e}^{\alpha \log(AB)}\\ &= \mathrm{e}^{\alpha(\log A + \log B - 2\pi \mathrm{i}\,\mathcal{U}(\log A + \log B))}\\ &= A^\alpha B^\alpha \mathrm{e}^{-2\alpha\pi \mathrm{i}\,\mathcal{U}(\log A + \log B)}. \qquad \square\end{aligned}$$

The Square Root Relation Explained

$$(1-z^2)^{1/2} = (1-z)^{1/2}(1+z)^{1/2}\,(-1)^{\mathcal{U}(\log(1-z)+\log(1+z))}.$$

Wlog, $\operatorname{Im} z \geq 0$. Then

$$\begin{aligned} 0 &\leq \arg(1+z) \leq \pi, \\ -\pi &\leq \arg(1-z) \leq 0, \end{aligned}$$

so

$$\begin{aligned} &\operatorname{Im}\bigl[\log(1-z)+\log(1+z)\bigr] \in (-\pi,\pi] \\ \Rightarrow\quad &\mathcal{U}\bigl[\log(1-z)+\log(1+z)\bigr] = 0. \end{aligned}$$

This is not true for $z-1$ and $z+1$!

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Early Definition

W. H. Metzler, *On the Roots of Matrices* (1892):

(d). *Sin*$^{-1}\phi$.—I define $\sin^{-1}\phi$ as follows:

$$\sin^{-1}\phi = \frac{\phi}{1} + \frac{1}{2}\cdot\frac{\phi^3}{3} + \frac{1.3}{2.4}\cdot\frac{\phi^5}{5} + \ldots\ldots + \frac{1.3\ldots\ldots\overline{2r-1}}{2.4\ldots\ldots 2r}\cdot\frac{x^{2r+1}}{2r+1} + \ldots\ldots$$

$$= \sum_0^\infty {}_\lambda \frac{1.3\ldots\ldots\overline{2\lambda-1}}{2.4\ldots\ldots 2\lambda}\cdot\frac{\phi^{2\lambda+1}}{2\lambda+1}.$$

- “Proves” $\sin(\operatorname{asin} A) = A$.

Application (1)

Household Consumption of Cheese: An Inverse Hyperbolic Sine Double-Hurdle Model with Dependent Errors

Steven T. Yen and Andrew M. Jones

The dependent double-hurdle model is generalized by an inverse hyperbolic sine transformation of the dependent variable. The resulting specification features a flexible parameterization, accommodates heteroskedastic errors, and nests a range of common limited dependent variable models. Results for U.S. household cheese

American Journal of Agricultural Economics, 1977

Application (2)

In a 1954 paper on the energy equation of a free-electron model :

Finally, let us define the "energy matrix" for the modified FE model:

$$\mathbf{E} = E_D[\arccos^2(\tfrac{1}{3}\mathbf{M}) - \tfrac{1}{4}\pi^2\mathbf{I}] + E^0\mathbf{I}, \qquad (2.18)$$

$$\mathbf{E} - E^0\mathbf{I} = E_D\pi[-(\tfrac{1}{3}\mathbf{M}) + (\tfrac{1}{3}\mathbf{M})^2/\pi - (\tfrac{1}{3}\mathbf{M})^3/6 + (\tfrac{1}{3}\mathbf{M})^4/3\pi\cdots], \qquad (2.19)$$

Toolbox of Matrix Functions

$$\frac{d^2y}{dt^2} + Ay = 0, \qquad y(0) = y_0, \quad y'(0) = y'_0$$

has solution

$$y(t) = \cos(\sqrt{A}\,t)y_0 + \left(\sqrt{A}\right)^{-1}\sin(\sqrt{A}\,t)y'_0.$$

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But

$$\begin{bmatrix} y' \\ y \end{bmatrix} = \exp\left(\begin{bmatrix} 0 & -tA \\ tI_n & 0 \end{bmatrix}\right)\begin{bmatrix} y_0' \\ y_0 \end{bmatrix}.$$

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- In software want to be able evaluate interesting f at matrix args as well as scalar args.

Existing Software

- MATLAB has built-in **`expm`**, **`logm`**, **`sqrtm`**, **`funm`**. We have written **`cosm`**, **`sinm`**, **`signm`**, **`powerm`**, **`lambertwm`**, **`unwindm`**, ...
- Julia has **`expm`**, **`logm`**, **`sqrtm`**.
- NAG Library has 42+ $f(A)$ codes.

H & Deadman, **A Catalogue of Software for Matrix Functions** (2016).

Definitions

$$\cos X = \frac{e^{iX} + e^{-iX}}{2}, \qquad \sin X = \frac{e^{iX} - e^{-iX}}{2i},$$

$$\cosh X = \cos iX, \qquad \sinh X = -i \sin iX.$$

- Concentrate on **inverse cosine**.
- Analogous results for inverse sine, inverse hyperbolic cosine, inverse hyperbolic sine.

- Joint work with Mary Aprahamian.

Inverse Cosine

$$A = \cos X = \frac{e^{iX} + e^{-iX}}{2},$$

implies

$$(e^{iX} - A)^2 = A^2 - I$$

or

$$e^{iX} = A + \sqrt{A^2 - I}.$$

Inverse Cosine

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implies

$$(e^{iX} - A)^2 = A^2 - I$$

or

$$e^{iX} = A + \sqrt{A^2 - I}.$$

But not all square roots give a solution!

Theorem

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

Problems

Pólya & Szegö, Problems and Theorems in Analysis II (1998): do

$$\sin X = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad \sin X = \begin{bmatrix} -1 & -1 \\ 0 & -1 \end{bmatrix}$$

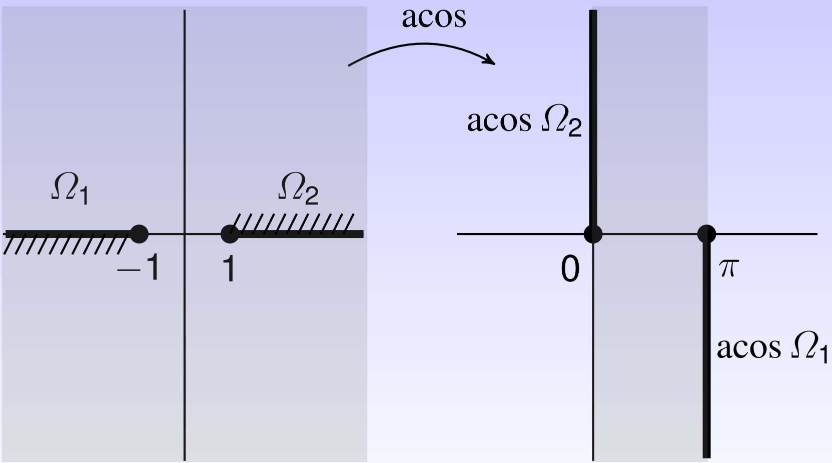
have a solution?

Putnam Problem 1996-B4: does

$$\sin X = \begin{bmatrix} 1 & 1996 \\ 0 & 1 \end{bmatrix}$$

have a solution?

Principal Inverse Cosine



Existence and Uniqueness

Theorem

If $A \in \mathbb{C}^{n\times n}$ has no ei'vals ± 1 there is a unique principal inverse cosine $\operatorname{acos} A$*, and it is a primary matrix function.*

Log Formula

Lemma

If $A \in \mathbb{C}^{n\times n}$ has no ei'vals ± 1,

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

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MATLAB docs *define* acos by first expression for scalars. Not obvious that RHS satisfies the conditions for acos!

- Is the lemma an immediate consequence of the scalar case?

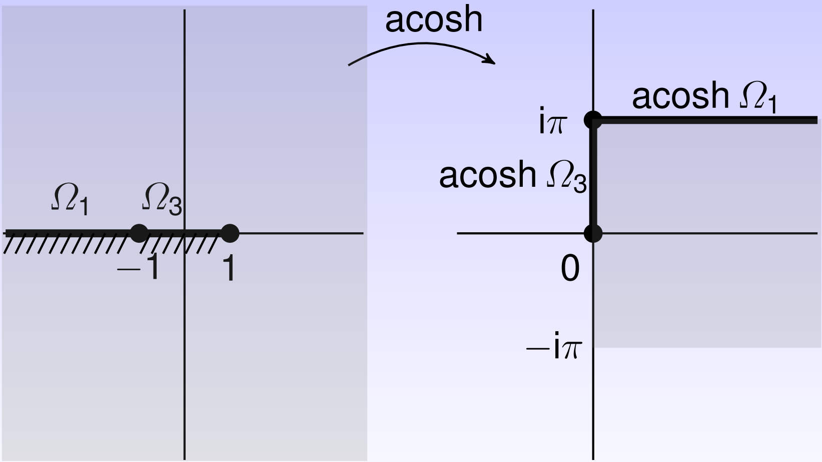
When Scalar Identity Implies Matrix Identity

Theorem (Horn & Johnson, 1991)

If $f \in C^{n-1}$ then $f(A) = 0$ for all $A \in \mathbb{C}^{n\times n}$ iff $f(z) = 0$ for all $z \in \mathbb{C}$.

- $\cos^2 A + \sin^2 A = I$ $\quad \surd$
- Not applicable for identities involving branch cuts.

Principal Inverse Coshine



acos and acosh

Abramowitz & Stegun: $\operatorname{acosh} z = \pm \mathrm{i} \operatorname{acos} z$.

Theorem

If $A \in \mathbb{C}^{n\times n}$ *has no ei'val* -1 *or on* $(0,1]$ *then*

$$\operatorname{acosh} A = \mathrm{i}\,\operatorname{sign}(-\mathrm{i}A)\,\operatorname{acos} A.$$

Sign is based on the scalar map

$$z \to \operatorname{sign}(\operatorname{Re} z) = \pm 1,$$
$$\operatorname{sign}(0) = 1,$$
$$\operatorname{sign}(y\mathrm{i}) = \operatorname{sign}(y) \text{ for } 0 \neq y \in \mathbb{R}.$$

Roundtrip Relations

- By definition, $\cos(\operatorname{acos} A) = A$.
- What about $\operatorname{acos}(\cos A) = A$?

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Theorem

If $A \in \mathbb{C}^{n\times n}$ has no ei'val with real part $k\pi$, $k \in \mathbb{Z}$, then

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

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Corollary

$\operatorname{acos}(\cos A) = A$ *iff every e'val of A has real part in* $(0, \pi)$.

Outline

GNU Octave

thfm ("Trigonometric/hyperbolic functions of square matrix")

Does not return the principal value of acosh! Uses

$$\operatorname{acosh} A = \log(A + (A^2 - I)^{1/2})$$

instead of

$$\operatorname{acosh} A = \log(A + (A - I)^{1/2}(A + I)^{1/2}).$$

Padé Approximation

Rational $r_{km}(x) = p_{km}(x)/q_{km}(x)$ is a $[k, m]$ **Padé approximant** to f if p_{km} and q_{km} are polys of degree at most k and m and

$$f(x) - r_{km}(x) = O(x^{k+m+1}).$$

- Generally more efficient than truncated Taylor series.
- Possible representations:
  - Ratio of polys.
  - Continued fraction.
  - Partial fraction.

Henri Padé
1863–1953

Padé Approximation for acos

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

Use **Padé approximants** of $f(x) = (2x)^{-1/2}\operatorname{acos}(1-x)$.
Backward error $h_m(A)$ defined by

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

satisfies

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

In fact, replace $\|A\|$ by $\alpha_p(A)$, where, with $p(p-1) \le 2m+1$,

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

Reducing the Argument

Use $\operatorname{acos} X = 2 \operatorname{acos}\big((\frac{1}{2}(I + X))^{1/2}\big)$ to get argument near I.

Lemma

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

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

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

- Not trivial to prove!
- Our proof: derive scalar result, then apply general result of Iannazzo (2007).

Choice of Padé Degree

- Take enough square roots to get close to I.
- Then balance cost of extra square roots with cost of evaluating r_m.
- Use fact that

$$(I - X_{k+1})(I + X_{k+1}) = I - X_{k+1}^2 = \frac{I - X_k}{2}$$

implies $\|I - X_{k+1}\| \approx \|I - X_k\|/4$.

Other Features

- Initial Schur decomposition.
- Compute square roots using Björck–Hammarling (1983) recurrence.
- Use *estimates* of $\|A^k\|_1$ (alg of H & Tisseur (2000)).
- Get the other functions from

$$\begin{aligned} \operatorname{asin} A &= (\pi/2)I - \operatorname{acos} A, \\ \operatorname{asinh} A &= \mathrm{i}\operatorname{asin}(-\mathrm{i}A) = \mathrm{i}\big((\pi/2)I - \operatorname{acos}(-\mathrm{i}A)\big), \\ \operatorname{acosh} A &= \mathrm{i}\operatorname{sign}(-\mathrm{i}A)\operatorname{acos} A. \end{aligned}$$

How to Test an Algorithm for $\operatorname{acos} A$?

Could check identities

- Roundtrip relations.
- $\operatorname{acos} A + \operatorname{asin} A = (\pi/2)I$.
- $\sin(\operatorname{acos} A) = (I - A^2)^{1/2}$.

Deadman & H (2016) give relevant "fudge factors".

Here, compute relative errors

$$\frac{\|X - \widehat{X}\|_1}{\|X\|_1},$$

where X computed at high precision using
$A = VDV^{-1} \Rightarrow f(A) = Vf(D)V^{-1}$ (**AdvanPix Toolbox**).

Comparison

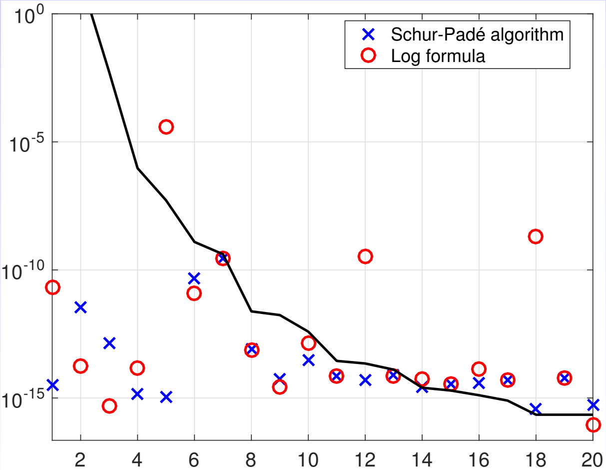
- **Schur–Padé alg** (Schur decomposition, square roots, Padé approximant).
- The formula

$$\operatorname{acos} A = -\mathrm{i} \log(A + \mathrm{i}(I - A^2)^{1/2})$$

computed with MATLAB **`logm`** and **`sqrtm`**, using a single Schur decomposition. GNU Octave uses this formula.

Experiment, $n = 10$

For acos, compare new alg with log formula



The Problem with the Log Formulas

$$\operatorname{acos} A = -\mathrm{i} \log(A + \mathrm{i}(I - A^2)^{1/2})$$

$$A = \begin{bmatrix} 0 & b \\ -b & 0 \end{bmatrix}, \quad b = 1000, \qquad \Lambda(A) = \{\pm 1000\,\mathrm{i}\}.$$

$$\frac{\|\operatorname{acos} A - \widehat{X}\|_1}{\|\operatorname{acos} A\|_1} \approx \begin{cases} 1.98 \times 10^{-9} & \text{log formula,} \\ 3.68 \times 10^{-16} & \text{new Alg.} \end{cases}$$

E'vals of $A + \mathrm{i}(I - A^2)^{1/2} \approx \{5 \times 10^{-5}\,\mathrm{i}, 2000\,\mathrm{i}\}$.

- Relative 1-norm condition number of $\operatorname{acos} A$ is 0.83.
- Instability of log formula.

Conclusions

First thorough treatment of inverse trigonometric and inverse hyperbolic matrix functions.

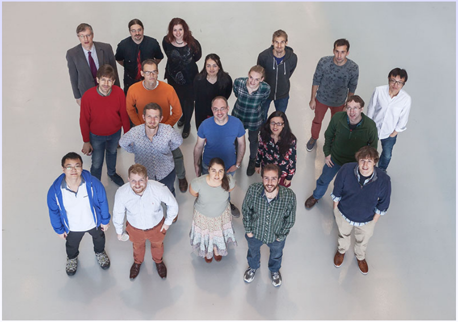
- Existence and uniqueness results.
- Various scalar identities extended to matrix case.
- New **roundtrip identities** (new even in scalar case).
- **New Schur–Padé algs**—numerically stable.
- MATLAB codes on GitHub: `https://github.com/higham/matrix-inv-trig-hyp`

Mary Aprahamian & H (2016), **Matrix Inverse Trigonometric and Inverse Hyperbolic Functions: Theory and Algorithms**, MIMS EPrint.

Future Directions

- Theory and algs for **non-primary** functions, perhaps linked to an $f(A(t))$ application.
- Better understanding of **conditioning** of $f(A)$.
- Matrix **argument reduction**.
- $f(A)b$ **problem**.

Manchester NLA group



References I

- Multiprecision Computing Toolbox.
  Advanpix, Tokyo.
  http://www.advanpix.com.
- A. H. Al-Mohy and N. J. Higham.
  Improved inverse scaling and squaring algorithms for the matrix logarithm.
  SIAM J. Sci. Comput., 34(4):C153–C169, 2012.
- T. M. Apostol.
  Mathematical Analysis.
  Addison-Wesley, Reading, MA, USA, second edition, 1974.
  xvii+492 pp.

References II

M. Aprahamian and N. J. Higham.
The matrix unwinding function, with an application to computing the matrix exponential.
SIAM J. Matrix Anal. Appl., 35(1):88–109, 2014.

R. M. Corless, J. H. Davenport, D. J. Jeffrey, and S. M. Watt.
"According to Abramowitz and Stegun" or arccoth needn't be uncouth.
ACM SIGSAM Bulletin, 34(2):58–65, 2000.

R. M. Corless and D. J. Jeffrey.
The unwinding number.
ACM SIGSAM Bulletin, 30(2):28–35, June 1996.

References III

- E. Deadman and N. J. Higham.
  Testing matrix function algorithms using identities.
  ACM Trans. Math. Software, 42(1):4:1–4:15, Jan. 2016.

- M. Fasi, N. J. Higham, and B. Iannazzo.
  An algorithm for the matrix Lambert W function.
  SIAM J. Matrix Anal. Appl., 36(2):669–685, 2015.

- N. J. Higham.
  Functions of Matrices: Theory and Computation.
  Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2008.
  ISBN 978-0-898716-46-7.
  xx+425 pp.

References IV

N. J. Higham and A. H. Al-Mohy.
Computing matrix functions.
Acta Numerica, 19:159–208, 2010.

N. J. Higham and E. Deadman.
A catalogue of software for matrix functions. Version 2.0.
MIMS EPrint 2016.3, Manchester Institute for Mathematical Sciences, The University of Manchester, UK, Jan. 2016.
22 pp.
Updated March 2016.

References V

N. J. Higham and F. Tisseur.
A block algorithm for matrix 1-norm estimation, with an application to 1-norm pseudospectra.
SIAM J. Matrix Anal. Appl., 21(4):1185–1201, 2000.

R. A. Horn and C. R. Johnson.
Topics in Matrix Analysis.
Cambridge University Press, Cambridge, UK, 1991.
ISBN 0-521-30587-X.
viii+607 pp.

References VI

B. Iannazzo.
Numerical Solution of Certain Nonlinear Matrix Equations.
PhD thesis, Università degli studi di Pisa, Pisa, Italy, 2007.
180 pp.

D. J. Jeffrey, D. E. G. Hare, and R. M. Corless.
Unwinding the branches of the Lambert W function.
Math. Scientist, 21:1–7, 1996.

References VII

W. Kahan.
Branch cuts for complex elementary functions or much ado about nothing's sign bit.
In A. Iserles and M. J. D. Powell, editors, *The State of the Art in Numerical Analysis*, pages 165–211. Oxford University Press, 1987.

W. H. Metzler.
On the roots of matrices.
Amer. J. Math., 14(4):326–377, 1892.

P. Penfield, Jr.
Principal values and branch cuts in complex APL.
SIGAPL APL Quote Quad, 12(1):248–256, Sept. 1981.

References VIII

G. Pólya and G. Szegö.
Problems and Theorems in Analysis II. Theory of Functions. Zeros. Polynomials. Determinants. Number Theory. Geometry.
Springer-Verlag, New York, 1998.
ISBN 3-540-63686-2.
xi+392 pp.
Reprint of the 1976 edition.

K. Ruedenberg.
Free-electron network model for conjugated systems. V. Energies and electron distributions in the FE MO model and in the LCAO MO model.
J. Chem. Phys., 22(11):1878–1894, 1954.

References IX

S. T. Yen and A. M. Jones.
Household consumption of cheese: An inverse hyperbolic sine double-hurdle model with dependent errors.
American Journal of Agricultural Economics, 79(1): 246–251, 1997.