Efficient Algorithms for the Matrix Cosine and Sine

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Matrix Cosine

$$\cos(A) = \sum_{i=0}^{\infty} \frac{(-1)^i}{(2i)!} A^{2i}, \qquad A \in \mathbb{C}^{n\times n}.$$

Application

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

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

Aims

- Compute $\cos(A)$ in IEEE double: maximal accuracy, minimal work.
- Compute $\cos(A)$ and $\sin(A)$ together.
- Preprocess data to reduce cost (not considered here).

Algorithm (H & Smith, 2003)

Serbin & Blalock (1980) propose rational approximations plus use of $\cos(2A) = 2\cos^2(A) - I$.

Algorithm 1 *Approximates* $X = \cos(A)$ *for* $A \in \mathbb{C}^{n\times n}$*.*

```
Find smallest m ≥ 0 s.t. 2^{-m}‖A‖_∞ ≤ 1.
C_0 = r_88(2^{-m} A)      % [8/8] Pade approximant
for i = 0: m − 1
    C_{i+1} = 2C_i^2 − I
end
X = C_m
```

H & Smith show that

$$\frac{\|\cos(A) - r_{88}(A)\|_\infty}{\|\cos(A)\|_\infty} \le 3.26 \times 10^{-16} \approx 3u \quad \text{for } \|A\|_\infty \le 1.$$

Truncation Analysis

$r_{2m}(x) = \dfrac{p_{2m}(x)}{q_{2m}(x)}$: $[2m/2m]$ Padé approximant of $\cos(x)$.

$$\cos(A) - r_{2m}(A) = \sum_{i=2m+1}^{\infty} c_{2i} A^{2i}$$

$$\Rightarrow \qquad \|\cos(A) - r_{2m}(A)\| \le \sum_{i=2m+1}^{\infty} |c_{2i}| \theta^{2i},$$

where $\theta = \theta(A) = \|A^2\|^{1/2}$.

$$\begin{aligned}\|\cos(A)\| &\ge 1 - \frac{\|A^2\|}{2!} - \frac{\|A^2\|^2}{4!} - \cdots = 1 - (\cosh(\|A^2\|^{1/2}) - 1) \\ &= 2 - \cosh(\theta).\end{aligned}$$

Relative Error Bound

$$\frac{\|\cos(A) - r_{2m}(A)\|}{\|\cos(A)\|} \le \frac{\sum_{i=2m+1}^{\infty} |c_{2i}|\theta^{2i}}{2 - \cosh(\theta)} \quad (\theta < \cosh^{-1}(2) \approx 1.317).$$

- For each $2m$ determine largest $\theta = \|A^2\|^{1/2}$ such that bound $\le u$.
- Compute c_{2i} symbolically, evaluate bound in high precision.

$2m$	2	4	6	8	10	12	14
θ_{2m}	6.1e-3	1.1e-1	4.3e-1	9.5e-1	1.315	1.317	1.317

Cost and Stability

Number of matrix mults to evaluate $p_{2m}(A)$ and $q_{2m}(A)$.

$2m$	2	4	6	8	10	12
Mults	1	2	3	4	5	5

Upper bound for $\kappa(q_{2m}(A))$ when $\theta \le \theta_{2m}$.

$2m$	2	4	6	8	12
Bound	1.0	1.0	1.0	1.0	1.1

- Choose strategy to minimize number of double-angle steps while minimizing the total work.

Variable Degree Padé Algorithm

Algorithm 2 *Approximates* $C = \cos(A)$ *for* $A \in \mathbb{C}^{n\times n}$.

$B = A^2$, $\theta = \|B\|_\infty^{1/2}$
for $d = [2\ 4\ 6\ 8\ 12]$
    if $\theta \le \theta_d$
        $C = r_d(A)$
        quit
    end
end
$s = \mathrm{ceil}(\log_2(\theta/\theta_{12}))$
$B \leftarrow 4^{-s}B$
if $\|B\|_\infty^{1/2} \le \theta_8$, $d = 8$, else $d = 12$, end
$C = r_d(2^{-s}A)$
for $i = 1\colon s$
    $C \leftarrow 2C^2 - I$
end

Error Analysis

Let $\widehat{C}_i =: C_i + E_i$. Can show that for Algs 1 and 2 $\|E_0\|_\infty \lesssim u\|C_0\|_\infty$, $\|C_0\|_\infty \le 2$, and

$$\|E_s\|_\infty \lesssim (4.1)^s u\|C_0\|_\infty\|C_1\|_\infty \dots \|C_{s-1}\|_\infty + nu\sum_{j=0}^{s-1} 4.1^{s-j-1}(2.21\|C_j\|_\infty^2 + 1)\|C_{j+1}\|_\infty \dots \|C_{s-1}\|_\infty.$$

- Same bounds hold with absolute bound $\|E_0\| \le u$.
- Effect of abs versus rel E_0 bound depends on $\|C_0\|, \dots, \|C_{s-1}\|$.
- Expect bound for $\|C_0\|$ larger for abs err criterion, but may permit fewer double-angle steps (smaller s).

Truncation Error and Stability

- Largest θ such that abs error bound $\leq u$:

$2m$	2	4	6	8	12	16	20
θ_{2m}	6.1e-3	0.11	0.43	0.98	2.6	4.7	7.1

- Upper bound for $\kappa(q_{2m}(A))$ for $\theta \leq \theta_{2m}$:

$2m$	2	4	6	8	10	12	14	16
Bound	1.0	1.0	1.0	1.0	1.1	1.2	1.4	1.8

- Logic for choice of scaling and $2m$ (once $\theta \leq \theta_{20}$):

Range of θ	d
$[0, \theta_{16}]$ = $[0, 4.7]$	smallest $d \in \{2, 4, 6, 8, 12, 16\}$ s.t. $\theta \leq \theta_d$
$(\theta_{16}, 2\theta_{12}]$ = $(4.7, 5.2]$	12 (scale by 1/2)
$(2\theta_{12}, \theta_{20}]$ = $(5.2, 7.1]$	20 (no scaling)

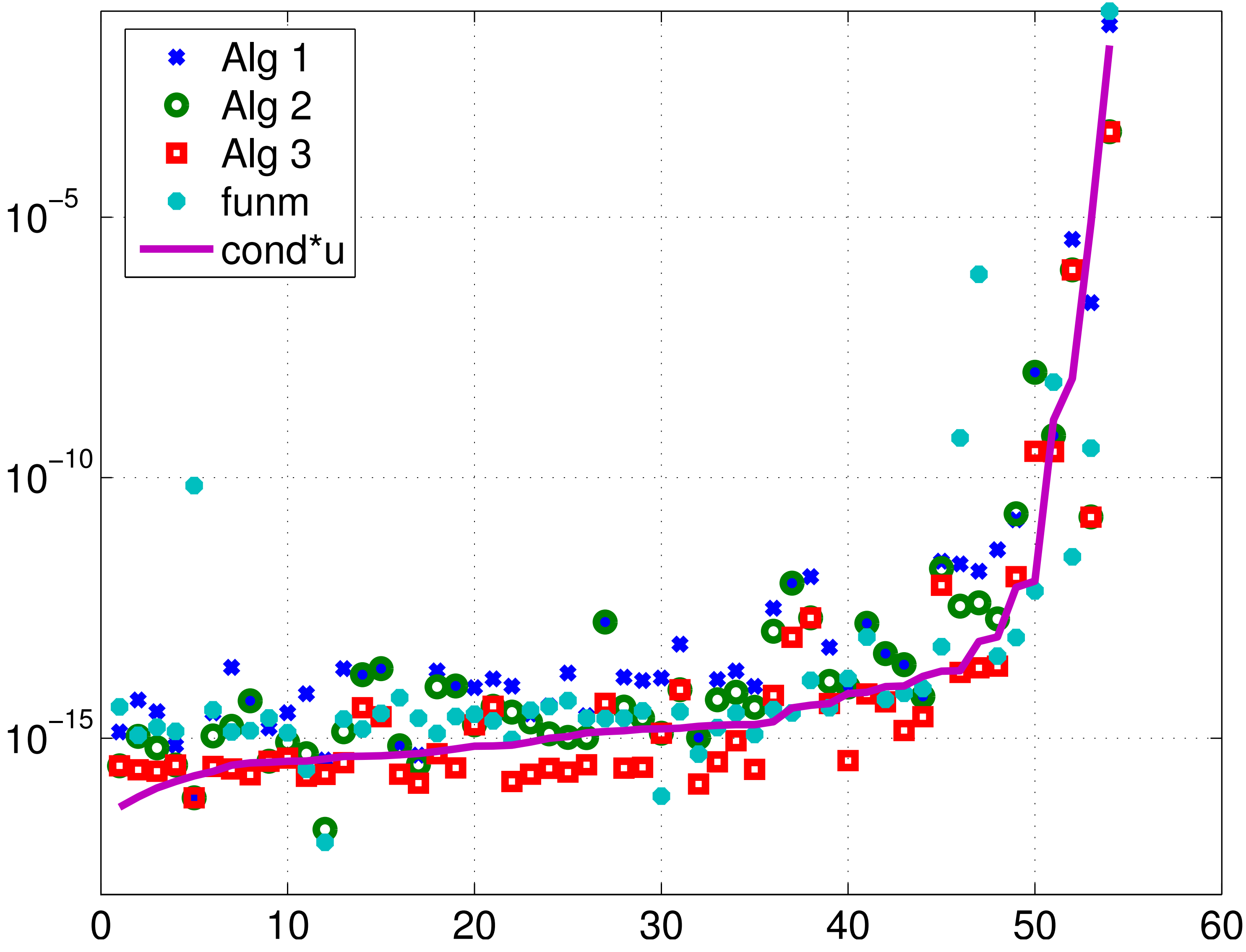
Absolute Error-Based Algorithm

Algorithm 3 *Approximates* $C = \cos(A)$ *for* $A \in \mathbb{C}^{n\times n}$.

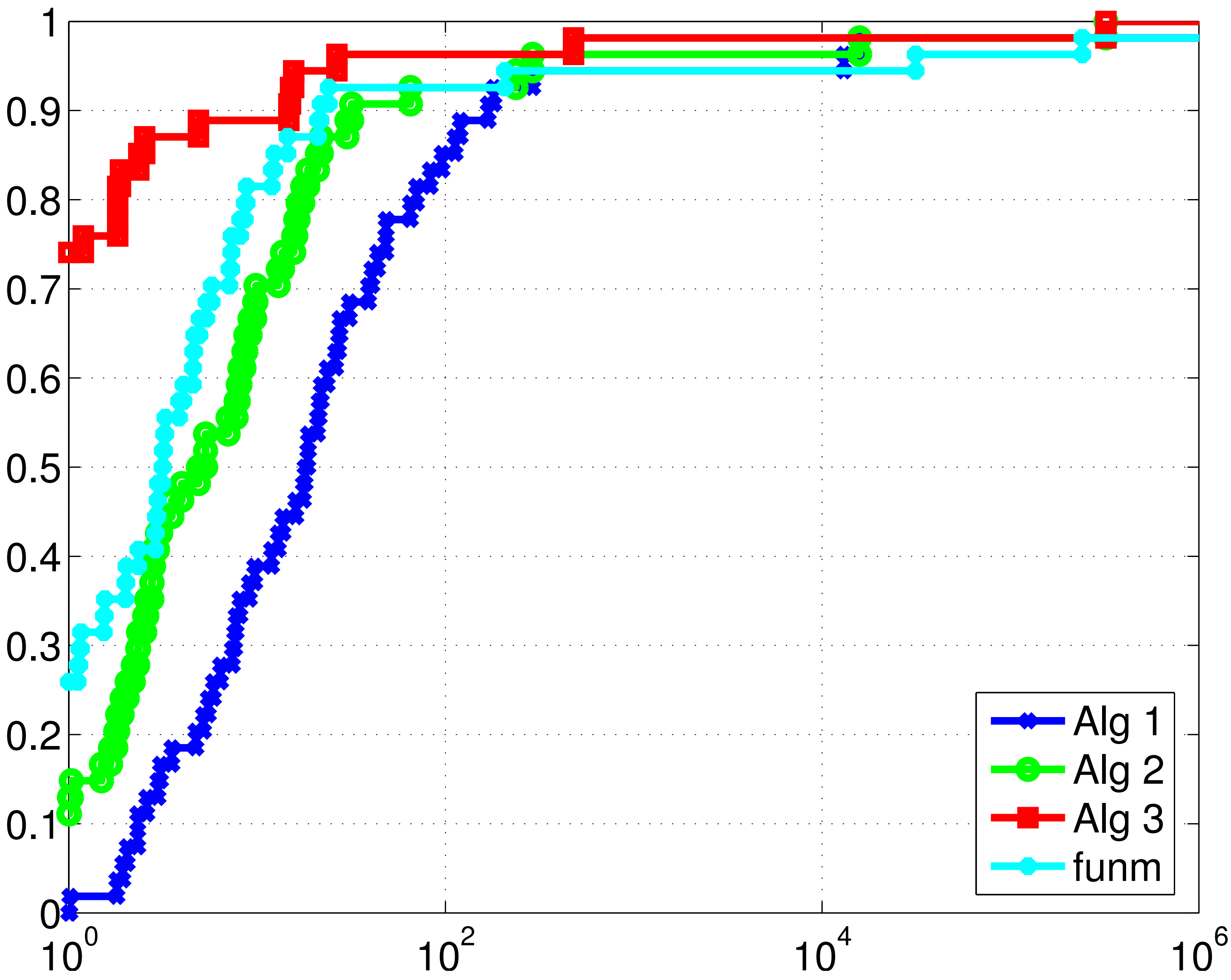
$B = A^2$, $\theta = \|B\|_\infty^{1/2}$
for $d = [2\ 4\ 6\ 8\ 12\ 16]$
    if $\theta \le \theta_d$
        $C = r_d(A)$
        quit
    end
end
$s = \mathrm{ceil}(\log_2(\theta/\theta_{20}))$
Determine optimal d from table; increase s as necessary.
$B \leftarrow 4^{-s}B$
$C = r_d(2^{-s}A)$
for $i = 1\colon s$
    $C \leftarrow 2C^2 - I$
end

Test 1: Relative Error

54 10×10 test matrices, norms 1–10^7.



Performance Profile



Cost Comparison

- `funm` requires a Schur decomposition.
  Costs between $28n^3$ and $n^4/3$ flops.
- Avge # matrix multiplies/solves for Algs 1–3 depends on $\|A^2\|$. Over the test set:

Alg 1	10
Alg 2	9.2
Alg 3	8.6

Computing Sine

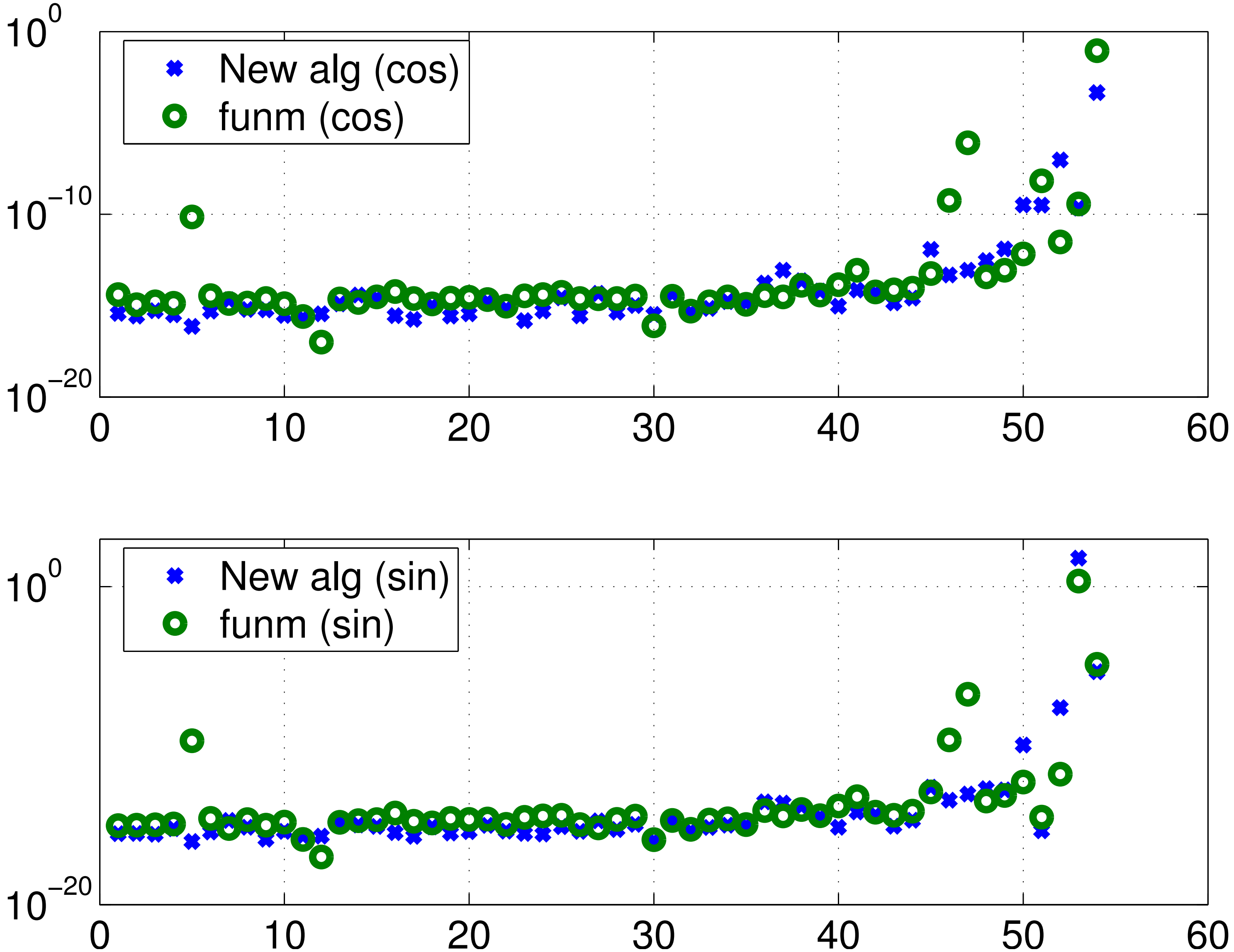
No analogue of above algs, since $\sin(2A) = 2\sin(A)\cos(A)$ requires cosines. So use $\sin(A) = \cos(A - \frac{\pi}{2}I)$.

Computing Sine and Cosine

- Scale so $\|2^{-s}A\| \leq \theta_{2m}$ and evaluate r_{2m} for cosine and $\widetilde{r}_{2m+1}$ for sine.
- Evaluating p_{2m}, q_{2m}, $\widetilde{p}_{2m+1}$ and $\widetilde{q}_{2m+1}$ reduces to evaluating four even polynomials of degree $2m$.
- Apply the double-angle formulas $\cos(2A) = 2\cos^2(A) - I$ and $\sin(2A) = 2\sin(A)\cos(A)$.

Sin/Cos Relative Error

54 10×10 test matrices, norms 1–10^7.



Conclusions

★ Improved on existing matrix cosine algs by

- using variable degree Padé approximants,
- basing truncation error bounds on $\theta(A) = \|A^2\|^{1/2}$ instead of $\|A\|$,
- minimizing work & # double angle steps,
- using absolute error criterion instead of relative.

★ Modification of alg permits simultaneous evaluation of $\cos(A)$ and $\sin(A)$.

G. I. Hargreaves and N. J. Higham.
Efficient algorithms for the matrix cosine and sine.
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