MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

A scaling and recovering algorithm for the matrix φ-functions

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The Matrix Exponential and φ-Functions

The most studied matrix function by far is the matrix exponential

$$e^A = I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots = \sum_{k=0}^{\infty} \frac{A^k}{k!};$$

see (Moler & Van Loan; '78, '03)

Nineteen dubious ways to compute the exponential of a matrix (1978); —, twenty-five years later (2003).

Closely related are the matrix φ-functions

$$\varphi_0(A) = e^A, \quad \varphi_j(A) = \sum_{k=0}^{\infty} \frac{A^k}{(k+j)!}.$$

▷ φ_j satisfy the recurrence relation

$$\varphi_j(A) = A\varphi_{j+1}(A) + \frac{1}{j!}I.$$

Applications in ODEs and Exponential Integrators

For $A \in \mathbb{C}^{n\times n}$, $y \in \mathbb{C}^n$, and $y(0) = y_0$ (**Minchev & Wright, '05**),

$$\frac{\mathrm{d}y}{\mathrm{d}t} = Ay \quad \Rightarrow \quad y(t) = \mathrm{e}^{tA}y_0,$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = Ay + b + ct \quad \Rightarrow \quad y(t) = \mathrm{e}^{tA}y_0 + t\varphi_1(tA)b + t^2\varphi_2(tA)c,$$

$$\vdots$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = Ay + g(t,y) \quad \Rightarrow \quad y(t) = \mathrm{e}^{tA}y_0 + \sum_{k=1}^{\infty} \varphi_k\left(tA\right) t^k g^{(k-1)}(0, y_0).$$

- A suitable truncation forms the basis of many exponential integrators.

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- A suitable truncation forms the basis of many exponential integrators.

E.g.: (nonautonomous) exponential Rosenbrock–Euler method (**Pope, '63**):

$$y_{n+1} = y_n + h\varphi_1(hJ_n)F(t_n, y_n) + h^2\varphi_2(hJ_n)\frac{\partial F}{\partial t}(t_n, y_n), \quad J_n = \frac{\partial F}{\partial y}(t_n, y_n),$$

where $F(t,y) \equiv Ay + g(t,y)$, $y_n \approx y(t_n)$, $t_n = nh$, and $h > 0$ stepsize.

Krylov-Based Exponential Integrators

Different types of exponential integrator schemes can be expressed as

$$\varphi_0(A)w_0 + \varphi_1(A)w_1 + \cdots + \varphi_p(A)w_p,$$

where w_j some vector, p relates to the exponential integrator order.

[Compute $\varphi_j(A)w_j$ by Krylov method]:

1. Initialize $v_1 = w_j/\|w_j\|_2$.
2. Build orthonormal basis $V_m = [v_1, v_2, \ldots, v_m]$ of $\mathcal{K}_m(A, w_j) = \mathrm{span}\{w_j, Aw_j, \ldots, A^{m-1}w_j\}$ via the Arnoldi process:
$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T.$$
3. Project $\varphi_j(A)w_j$ onto a lower-dim. subspace (**Hochbruck & Lubich, '97**):
$$\varphi_j(A)w_j \approx \frac{\|w_j\|_2}{2\pi \mathrm{i}} \int_\Gamma \varphi_j(\sigma) V_m(\sigma I - H_m)^{-1} e_1 \mathrm{d}\sigma = \|w_j\|_2 V_m \varphi_j(H_m) e_1.$$

▷ Accurately and stably computing $\varphi_j(H_m)$ a key and challenging step.

Theorem (Lu, '03; Higham, '08)

$$B = \begin{bmatrix} A & I \\ 0 & 0 \end{bmatrix} \in \mathbb{C}^{2n\times 2n} \quad \Rightarrow \quad \mathrm{e}^{B} = \begin{bmatrix} \mathrm{e}^{A} & \varphi_1(A) \\ 0 & I \end{bmatrix}.$$

Evaluating φ-Functions from Exponentiation

Theorem (Lu, '03; Higham, '08)

$$B = \begin{bmatrix} A & I \\ 0 & 0 \end{bmatrix} \in \mathbb{C}^{2n\times 2n} \quad \Rightarrow \quad \mathrm{e}^B = \begin{bmatrix} \mathrm{e}^A & \varphi_1(A) \\ 0 & I \end{bmatrix}.$$

Theorem (Al-Mohy & L., '25)

Let $E = \begin{bmatrix} I & 0 & 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{n\times np}$ *and* $J = J_p(0) \otimes I$ *(*$J_p(0)$ *is* $p \times p$ *Jordan block associated with zero). Then*

$$W = \begin{bmatrix} A & E \\ 0 & J \end{bmatrix} \in \mathbb{C}^{(p+1)n\times(p+1)n} \Rightarrow f(W) = \begin{bmatrix} f(A) & g_1(A) \ \dots \ g_p(A) \\ 0 & f(J_p(0)) \otimes I \end{bmatrix},$$

where $g_i(A) = Ag_{i+1}(A) + f^{(i)}(0)I/i!, \quad g_0 = f, \quad i = 0\colon p-1.$

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where $g_i(A) = Ag_{i+1}(A) + f^{(i)}(0)I/i!, \quad g_0 = f, \quad i = 0\colon p-1.$

$\rightsquigarrow$ Corollary: setting $f = \exp \ \Rightarrow \ g_1(A) = \varphi_1(A), \dots, g_p(A) = \varphi_p(A)$.

- Approximate the first block row of e^W *without* forming W?

Theorem (Al-Mohy & L., '25)

The $[m+p-j/m]$ *Padé approximants to* $\varphi_j(z)$, $\mathcal{R}_{m+p-j,m}(z) =: \mathcal{R}_m^{(j)}(z)$, $j = 1\colon p$, *satisfy the recurrence relation*

$$\mathcal{R}_m^{(j)}(z) = z\mathcal{R}_m^{(j+1)}(z) + \frac{1}{j!}, \quad j = p-1\colon -1\colon 0.$$

Idea of proof: set f as the $[m+p/m]$ Padé approximant, $\mathcal{R}_m^{(0)}(z)$, to e^z.

• Adapt the Padé approximant degree per φ_j and fix the denominator in the construction.

$\rightsquigarrow$ Comput'nal advantage over evaluating fixed-deg. Padé approximants to φ-functions *independently*, avoiding repeated rational approximations.

Scaling and Squaring (Recovering) Method

For the matrix exponential: $\mathrm{e}^A = (\mathrm{e}^{2^{-s}A})^{2^s} \approx r_m(2^{-s}A)^{2^s}$

1 $B \leftarrow A/2^s$ so $\|B\|_1$ is close to the origin. ▷ scaling
2 Evaluate the $[m/m]$ Padé approximant $r_m(B)$ to e^B. ▷ evaluate
3 $\mathrm{e}^A \approx r_m(B)^{2^s}$ ▷ squaring

- Proposed by Lawson **(Lawson, '67)**.
- Algorithm, with rounding error analysis and a posteriori error bound **(Ward, '77)**.
- Backward truncation error analysis allowing choice of s and m **(Moler & Van Loan, '78)**.
- Sharper b'ward trunc. analysis giving optimal s and m minimizing computational cost in double precision **(Higham, '05)**.
- B'ward trunc. bound based on $\|A^k\|^{1/k}$ rather than $\|A\|$, alleviating overscaling issues **(Al-Mohy & Higham, '09)**, current MATLAB `expm`.

Simultaneously for the φ-functions: $\varphi_0(A) = \mathrm{e}^A$, $\varphi_1(A)$, $\dots$, $\varphi_p(A)$

Select a scaling parameter s and a degree m of Padé approximant.

$A \leftarrow A/2^s$

Evaluate the $[m/m]$ Padé approximant, $\mathcal{R}_m^{(p)}(A)$, to $\varphi_p(A)$.

Invoke the recurrence $\mathcal{R}_m^{(j)}(A) = A\mathcal{R}_m^{(j+1)}(A) + \frac{1}{j!}I$, $j = p-1 : -1 : 0$.

for $i = 1 : s$ **do**

    for $j = p : -1 : 0$ **do**

        $\mathcal{R}_m^{(j)}(A) \leftarrow 2^{-j}\left(\mathcal{R}_m^{(0)}(A)\mathcal{R}_m^{(j)}(A) + \sum_{k=1}^{j} \mathcal{R}_m^{(k)}(A)/(j-k)!\right)$

    end

end

- The double-argument formula $\varphi_j(2A) = \frac{1}{2^j}\left(\varphi_0(A)\varphi_j(A) + \sum_{k=1}^{j} \frac{\varphi_k(A)}{(j-k)!}\right)$ **(Berland, Skaflestad, Wright; '07)** for recov. $\varphi_j(A)$ from $\varphi_j(2^{-s}A)$, $j = 0 : p$.

$\rightsquigarrow$ Determine s and m to *guarantee accuracy* and *minimize comput'nal cost*.

Truncation Error Analysis [1/4]

Key: Set f as the $[m+p/m]$ Padé approximant, $\mathcal{R}_m^{(0)}(z)$, to e^z:

$$W = \begin{bmatrix} A & E \\ 0 & J \end{bmatrix} \quad \Rightarrow \quad \mathcal{R}_m^{(0)}(W) = \begin{bmatrix} \mathcal{R}_m^{(0)}(A) & \mathcal{R}_m^{(1)}(A) \ \ldots \ \mathcal{R}_m^{(p)}(A) \\ 0 & \mathcal{R}_m^{(0)}(J) \end{bmatrix}.$$

- Evaluation starts from the $[m/m]$ Padé approximant, $\mathcal{R}_m^{(p)}(A)$, to $\varphi_p(A)$, truncation error analysis based on $\mathcal{R}_m^{(0)}(A)$ to e^A. Let **(Higham, '08)**

$$h_{m,p}(A) = \log(\mathrm{e}^{-A}\mathcal{R}_m^{(0)}(A)) = \sum_{k=2m+p+1}^{\infty} c_{m,p,k}A^k,$$

then $\mathcal{R}_m^{(0)}(A) = \mathrm{e}^{A+h_{m,p}(A)}$. Hence

$$\left[\mathcal{R}_m^{(0)}(2^{-s}A)\right]^{2^s} = \mathrm{e}^{A+2^s h_{m,p}(2^{-s}A)} =: \mathrm{e}^{A+\Delta A},$$

and $\Delta A = 2^s h_{m,p}(2^{-s}A)$ represents the *backward error* resulting from approximating e^A via scaling and squaring.

Truncation Error Analysis [2/4]

The selected s need satisfy

$$\frac{\|\Delta A\|_1}{\|A\|_1} = \frac{2^s \|h_{m,p}(2^{-s}A)\|_1}{\|A\|_1} = \frac{\|h_{m,p}(2^{-s}A)\|_1}{\|2^{-s}A\|_1} \leq u \approx 1.1 \times 10^{-16}.$$

Computing *implicitly* $\exp\left(\begin{bmatrix} A+\Delta A & E+\Delta E \\ 0 & J+\Delta J \end{bmatrix}\right)$, what about ΔE?

Use the linear operator $\mathcal{D}_f(A, B, E)$ in (**Al-Mohy, '25**):

$$f\left(\begin{bmatrix} A & E \\ 0 & B \end{bmatrix}\right) = \begin{bmatrix} f(A) & \mathcal{D}_f(A,B,E) \\ 0 & f(B) \end{bmatrix}.$$

$\Delta E = \mathcal{D}_{h_{m,p}}(2^{-s}A, 2^{-s}J, E) = (1,2)$ block of $2^s h_{m,p}\left(\begin{bmatrix} 2^{-s}A & 2^{-s}E \\ 0 & 2^{-s}J \end{bmatrix}\right)$.

$\rightsquigarrow$ Invoke the theorem with $f = 2^s h_{m,p}$.

Truncation Error Analysis [3/4]

The jth block of ΔE is

$$(\Delta E)_j \;=\; 2^s A^{-j} h_{m,p}(2^{-s}A), \quad 1 \le j \le p.$$

Therefore, select s such that

$$\frac{\|\Delta E\|_1}{\|E\|_1} = \|\Delta E\|_1 \le \max_{1\le j\le p} \|(2^{-s}A)^{-j} h_{m,p}(2^{-s}A)\|_1 \le \max_{1\le j\le p} \frac{\widetilde{h}_{m,p}(\theta)}{\theta^j} \le u.$$

$\widetilde{h}_{m,p}(\theta) = \sum_{k=2m+p+1}^{\infty} |c_{m,p,k}|\theta^k$, $\theta \ge 0$ real-valued function of $2^{-s}A$.

- A simple choice for θ is $\|2^{-s}A\|_1$ (**Higham, '08**)

$$\Rightarrow \; \left\| \sum_{k=2m+p+1}^{\infty} |c_{m,p,k}|(2^{-s}A)^{k-j} \right\| \le \sum_{k=2m+p+1}^{\infty} |c_{m,p,k}| \|2^{-s}A\|_1^{k-j}.$$

- Idea: symbolically compute $c_{m,p,k}$ and find the scaling threshold

$$\theta_{m,p} = \max\{\, \theta : \max_{1\le j\le p} \widetilde{h}_{m,p}(\theta)/\theta^j \le u \approx 1.1 \times 10^{-16} \,\}.$$

Truncation Error Analysis [4/4]

Using $\theta = \alpha_r(2^{-s}A)$ (not $\|2^{-s}A\|_1$) leads to sharper bound (**Al-Mohy & Higham, '09**):

$$\alpha_r(A) = \min_{2\le r\le r_{\max}} \max\left(\|A^r\|_1^{1/r}, \|A^{r+1}\|_1^{1/(r+1)}\right).$$

- Motivation:

$$\rho(A) \le \|A^r\|^{1/r} \le \|A\|, \quad r = 1\colon \infty,$$

$\rho(A) \ll \|A\|$ for highly non-normal A, and $\lim_{r\to\infty} \|A^r\|^{1/r} = \rho(A)$.

$\rightsquigarrow$ $\|A^r\|^{1/r}$ instead of $\|A\|$ in bounding $\|\sum_{k=2m+p+1}^{\infty} |c_{m,p,k}|(2^{-s}A)^{k-j}\|$.

The *overall* relative b'ward errors are bounded by

$$\max\left(\frac{\|\Delta A\|_1}{\|A\|_1}, \frac{\|\Delta E\|_1}{\|E\|_1}\right) \le \frac{\widetilde{h}_{m,p}(\alpha_r(2^{-s}A))}{\alpha_r(2^{-s}A)^{\delta}} \le u, \quad \delta = 1 \text{ or } p.$$

- Need choose optimal s and m s.t. $2^{-s}\alpha_r(A) \le \theta_{m,p}$ for $2 \le r \le r_{\max}$.

Table of the Scaling Threshold $\theta_{m,p}$

Table: Selected values of $\theta_{m_i,p}$, at optimal Paterson–Stockmeyer degrees m_i.

p	$m_0 = 1$	$m_1 = 2$	$m_2 = 3$	$m_3 = 4$	$m_4 = 6$	$m_5 = 8$	$m_6 = 10$	$m_7 = 12$
1	2.00e-5	3.81e-3	3.97e-2	1.54e-1	7.26e-1	1.76	3.17	4.87
2	3.76e-5	6.09e-3	5.81e-2	2.13e-1	9.28e-1	2.06	3.54	5.28
3	7.37e-5	9.87e-3	8.53e-2	2.94e-1	1.16	2.37	3.91	5.69
4	1.50e-4	1.62e-2	1.26e-1	4.06e-1	1.40	2.69	4.28	6.09
5	3.15e-4	2.70e-2	1.87e-1	5.62e-1	1.66	3.01	4.65	6.50
6	6.86e-4	4.55e-2	2.80e-1	7.79e-1	1.92	3.34	5.02	6.90
7	1.54e-3	7.75e-2	4.18e-1	1.05	2.20	3.68	5.40	7.30
8	3.54e-3	1.33e-1	6.26e-1	1.26	2.48	4.01	5.77	7.69
9	8.35e-3	2.30e-1	9.34e-1	1.48	2.77	4.35	6.14	8.08
10	2.01e-2	3.99e-1	1.16	1.71	3.07	4.69	6.51	8.47

- Scale A down by 2^s such that $2^{-s}\alpha_r(A) \leq \theta_{m,p}$. Larger $m \rightsquigarrow$ higher threshold $\theta_{m,p}$ and less strong scaling needed.

Next: choose *feasible* s and m to minimize the computational cost.

Minimizing the Computational Cost

Select a scaling parameter s and a degree m of Padé approximant.
$A \leftarrow A/2^s$
Evaluate the $[m/m]$ Padé approximant, $\mathcal{R}_m^{(p)}(A)$, to $\varphi_p(A)$.
Invoke the recurrence $\mathcal{R}_m^{(j)}(A) = A\mathcal{R}_m^{(j+1)}(A) + \frac{1}{j!}I$, $j = p-1:-1:0$.
for $i = 1: s$ **do**
    for $j = p: -1 : 0$ **do**
        $\mathcal{R}_m^{(j)}(A) \leftarrow 2^{-j}\left(\mathcal{R}_m^{(0)}(A)\mathcal{R}_m^{(j)}(A) + \sum_{k=1}^{j}\mathcal{R}_m^{(k)}(A)/(j-k)!\right)$
    end
end

Total cost is

$$C_{m_i,s} = i + p + \frac{4}{3} + s(p+1),$$

where $s = \max\left(\lceil \log_2(\alpha_r(A)/\theta_{m,p}) \rceil, 0\right)$ s.t. $2^{-s}\alpha_r(A) \le \theta_{m,p}$.

$\rightsquigarrow$ Cost minimized over the index pair (m_i, r), $m_i \le m_{\max} = 12$ s.t. $\kappa(D_{m_i}(A))$ modest, $2 \le r \le r_{\max}$, $r_{\max}$ determined when $m_{\max}$ fixed.

Experimental setup

Algorithms:

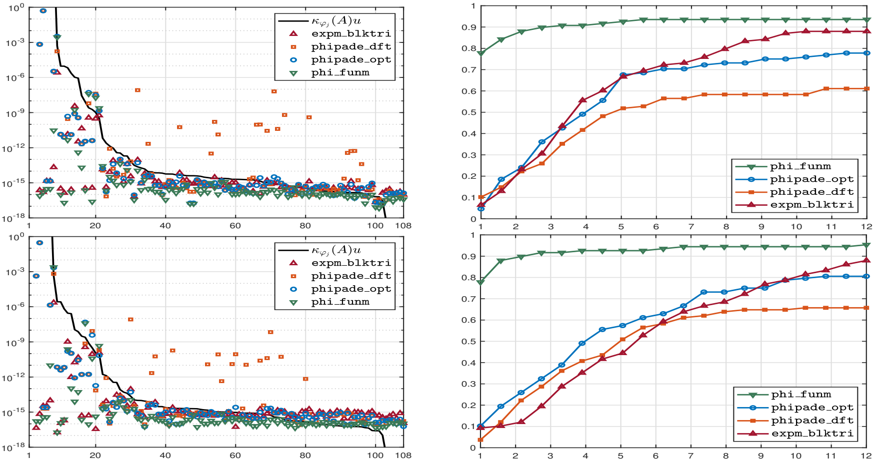
- `phi_funm`: the proposed algorithm;
- `phipade`: from EXPINT (**Berland, Skaflestad, Wright; '07**), realizing the algorithm (**Skaflestad & Wright, '09**) executed in two configurations:
  - `phipade_dft`: the default setting: uses the $[7/7]$ Padé approximant;
  - `phipade_opt`: the adaptive setting proposed in (**Skaflestad & Wright, '09**), seeking the optimal Padé degree $3 \leq m \leq 13$ to minimize the cost;
- `expm_blktri`: the algorithm of (**Al-Mohy, '25**), for computing the exp of block triangular matrices. (Comput. $(1, 2)$ block of e^{W} implicitly, not structure aware.)

Test set:

- 108 *nonnormal* matrices from matrix function literature, $2 \leq n \leq 41$.
- 5 Hessenberg matrices ($m = 30$, 80) from Arnoldi within Krylov methods for comput. $\varphi_j(A)e$, $e =$ `ones(n,1)`, $900 \leq n \leq 392{,}257$.

Working precision: binary64 (IEEE double) in MATLAB

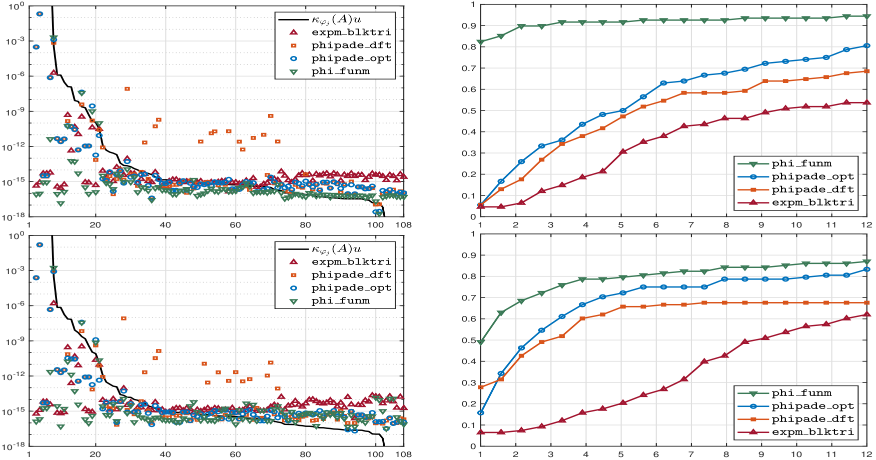
Accuracy and Stability: I



Top: $j = 1$; bottom: $j = 4$.

- $p = 10$. Left: 1-norm forward error. Right: performance profiles: fraction of tests whose relative error is within factor (x-axis) of the smallest.

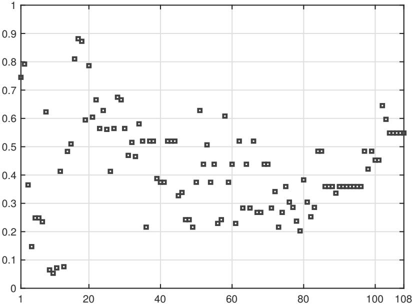
Accuracy and Stability: II



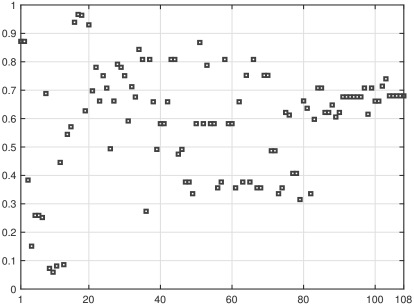
Top: $j = 7$; bottom: $j = 10$.

- phipade_dft unstable (overscaling), expm_blktri worsen as j grows.

Asymptotic Computational Cost



(a) `phi_funm` over `phipade_dft`.

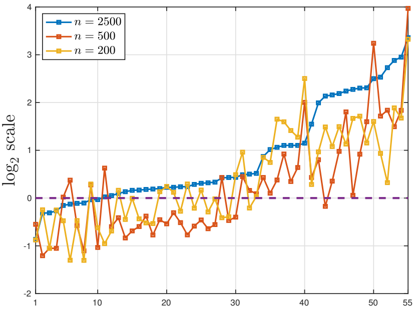


(b) `phi_funm` over `phipade_opt`.

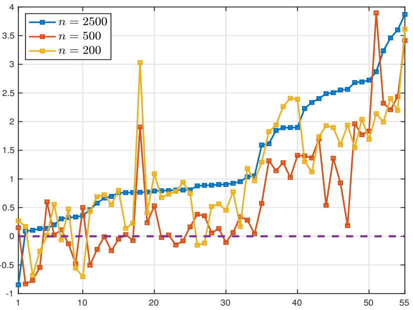
Figure: Ratios of computational cost: `phi_funm` to `phipade`.

- `phi_funm` *always* more efficient, can be $10\times$ to $20\times$ cheaper:
  - based on $\alpha_r(A)$ rather than $\|A\|_1 \rightsquigarrow$ less prone to overscaling.
  - adapts the Padé degree per $\varphi_j \rightsquigarrow$ saves at least p multiple linear-system solvers.

Runtime Comparison



(a) phi_funm vs phipade_dft.



(b) phi_funm vs phipade_opt.

Figure: $\log_2$-speedup of phi_funm to phipade. $y \geq 0$ indicate phi_funm is faster.

- For $n = O(100)$, phi_funm and phipade comparable in speed.
- Lower asymptotic cost of phi_funm reflected in runtime as n grows.
- phi_funm more *reliable*: runtimes $\lesssim 2\times$ the fastest, $16\times$ for phipade.

Hessenberg Matrices from Krylov Methods

		bcspwr10		gr_30_30		helm2d03		orani678		poisson99	
$p=1$		Error	Cost	Error	Cost	Error	Cost	Error	Cost	Error	Cost
$m=30$	phi_funm	3.2e-15	11.3	1.0e-15	12.3	1.4e-15	12.3	3.7e-16	8.3	7.5e-14	34.3
	phipade_dft	5.3e-9	14.7	1.1e-9	16.7	1.9e-10	16.7	5.7e-16	14.7	8.2e-14	38.7
	phipade_opt	2.0e-15	13.7	3.3e-15	15.7	2.1e-15	15.7	7.4e-16	13.7	7.8e-14	35.7
$m=80$	phi_funm	3.2e-15	11.3	1.0e-15	12.3	1.5e-15	12.3	4.9e-16	8.3	9.1e-14	34.3
	phipade_dft	5.3e-9	14.7	3.4e-14	18.7	1.9e-10	16.7	6.4e-16	18.7	1.1e-13	38.7
	phipade_opt	2.0e-15	13.7	1.8e-15	15.7	2.1e-15	15.7	9.8e-16	15.7	9.9e-14	35.7
$p=4$		Error	Cost	Error	Cost	Error	Cost	Error	Cost	Error	Cost
$m=30$	phi_funm	1.1e-15	16.3	8.2e-15	17.3	4.0e-15	17.3	6.8e-16	10.3	1.5e-14	72.3
	phipade_dft	5.0e-10	27.7	1.1e-9	32.7	1.8e-10	32.7	3.6e-16	27.7	5.4e-14	87.7
	phipade_opt	1.3e-15	23.7	3.1e-15	28.7	1.9e-15	28.7	4.5e-16	23.7	5.2e-14	78.7
$m=80$	phi_funm	1.1e-15	16.3	8.8e-15	17.3	4.1e-15	17.3	8.6e-16	10.3	2.0e-14	72.3
	phipade_dft	5.0e-10	27.7	3.3e-14	37.7	1.8e-10	32.7	1.3e-15	37.7	6.4e-14	87.7
	phipade_opt	1.3e-15	23.7	1.6e-15	28.7	1.9e-15	28.7	1.1e-15	28.7	5.9e-14	78.7

- phi_funm always has lower *computational cost*. Execution times comparable between 10^{-3} and 10^{-2} seconds (not shown).
- phi_funm and phipade_opt deliver good and comparable accuracy, but phipade_dft again shows *instability*.

Conclusions

Faster, **more accurate**, **b'ward stable** algorithm for **matrix φ-functions**:

- New recurrence between non-diagonal Padé approximants to $\varphi_j \rightsquigarrow$ Avoid repeated rational approximations $\rightsquigarrow$ Computational savings.
- Rigorous b'ward error analysis, $\rightsquigarrow$ Sharp relative error bounds & Proposed algorithm b'ward stable in *exact* arithmetic.
- Algorithmic parameters selected on the fly in $O(n^2)$ to minimize the overall computational cost.
- Matrix triangularity exploitation (not shown) by recomput. diagonals of $\varphi_0(A) = \mathrm{e}^A$ via explicit formulae $\rightsquigarrow$ Controlled error propagation.

▶ A. H. Al-Mohy and X. Liu. A scaling and recovering algorithm for the matrix φ-functions. SIAM J. Sci. Comput., To appear. Currently available at https://arxiv.org/abs/2506.01193.

Code available at https://github.com/xiaobo-liu/phi_funm

Next?

- Excellent *numerical* f'ward stability observed. Rounding error analysis?

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