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FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
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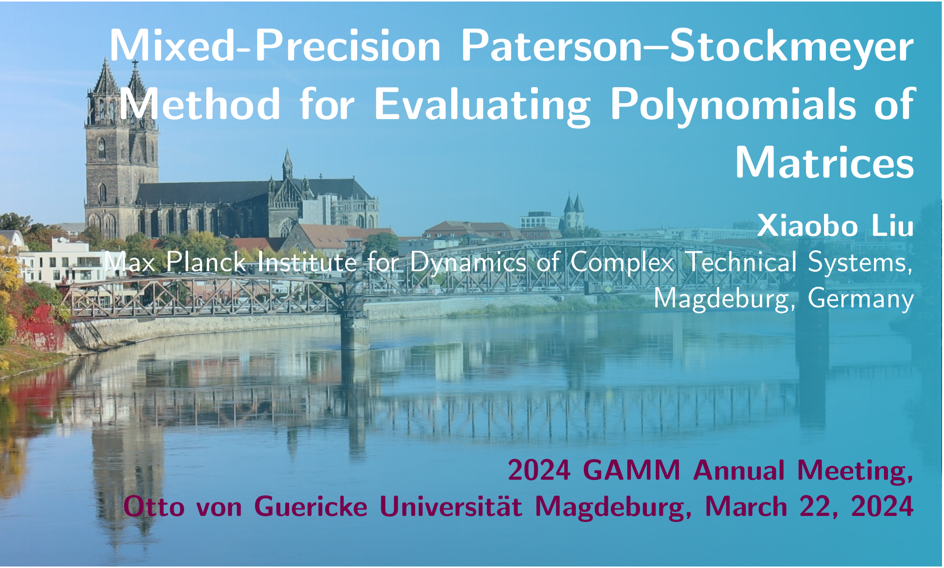
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY



Mixed-Precision Paterson–Stockmeyer Method for Evaluating Polynomials of Matrices

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Matrix Polynomials

The object and Motivation

The goal is to evaluate the matrix polynomial

$$p_m(X) = \sum_{i=0}^{m} b_i X^i = b_0 I + b_1 X + b_2 X^2 + \cdots + b_m X^m.$$

It often results from truncated series expansions (with $\|b_m X^m\| \leq \epsilon \ll 1$) in computation of matrix functions and solution of matrix equations:

- series expansion (e.g., Taylor series)
- rational functions $q(X)^{-1} p(X)$
- rational matrix equations $r(X) = A$

So, practically,

- $m \in \mathbb{N}$,
- $b_i \in \mathbb{C}$ and $|b_i|$ can decay quickly, e.g., the Taylor series of $\exp$, $\cos$
- $X \in \mathbb{C}^{n\times n}$ with $\|X\|$ usually being small.

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Paterson–Stockmeyer Method

For $s \in \mathbb{N}^{+}$, we can rewrite $p_m(X)$ as a polynomial in X^s with matrix coefficients B_i **(Paterson and Stockmeyer, 1973)**

$$p_m(X) = \sum_{i=0}^{r} B_i \cdot (X^s)^i, \quad r = \lfloor m/s \rfloor,$$

where

$$B_i = \begin{cases} \displaystyle\sum_{j=0}^{s-1} b_{si+j} X^j, & i = 0, \dots, r-1, \\ \displaystyle\sum_{j=0}^{m-sr} b_{sr+j} X^j, & i = r. \end{cases}$$

- For example, with $m = 6$ and $s = 3$,

$$p_6(X) = \underbrace{b_6 I}_{B_2} (X^3)^2 + \underbrace{(b_5 X^2 + b_4 X + b_3 I)}_{B_1} X^3 + \underbrace{(b_2 X^2 + b_1 X + b_0 I)}_{B_0}$$

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Paterson–Stockmeyer Method

Evaluation

$$p_m(X) = \Big(\big((B_r X^s + B_{r-1})X^s + B_{r-2}\big)X^s + \cdots + B_1\Big)X^s + B_0$$

```
Input  : $X \in \mathbb{C}^{n\times n}$, $b_0, b_1, \dots, b_m \in \mathbb{C}$
Output: $Z = p_m(X)$
$\mathcal{X}_0 \leftarrow I$, $\mathcal{X}_1 \leftarrow X$
for $i \leftarrow 2$ to $s$ do
    $\mathcal{X}_i \leftarrow X\mathcal{X}_{i-1}$        ▷ $X^2, \dots, X^s$ computed and stored
$Z \leftarrow \sum_{j=0}^{m-sr} b_{sr+j}\mathcal{X}_j$
for $i \leftarrow r-1$ down to $0$ do
    $Z \leftarrow Z\mathcal{X}_s + \sum_{j=0}^{s-1} b_{si+j}\mathcal{X}_j$
return $Z$
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- Two extreme cases: (i) $s = 1$: (plain) Horner's method
  (ii) $s = m$: evaluation via explicit powers.

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Paterson–Stockmeyer Method

Storage Requirement and Cost

$$p_m(X) = \Big(\big((B_r X^s + B_{r-1})X^s + B_{r-2}\big)X^s + \cdots + B_1\Big)X^s + B_0$$

- $(s+2)n^2$ elements of storage
- about $s-1+r$ matrix products, incl. $r = \lfloor m/s \rfloor$ products in the Horner's stage

Theorem (Hargreaves, 2005; Fasi, 2019)

The choice $s = \lfloor \sqrt{m} \rfloor$ or $s = \lceil \sqrt{m} \rceil$ minimizes the number of matrix products required to evaluate $p_m(A)$ over all choices of s. The minimized number of matrix products is about $2\sqrt{m}$.

Exploiting Multi-Precisions in Paterson–Stockmeyer

Observation and Key Idea

For $p_m(X) = \Big(\big((B_r X^s + B_{r-1})X^s + B_{r-2}\big)X^s + \cdots + B_1\Big)X^s + B_0$,
$\|B_i\|\,\|X^s\| \ll \|B_{i-1}\|$ can hold for some $i = v\colon r$,

$$\Big\|b_{si}I + b_{si+1}X + \cdots + b_{si+s-1}X^{s-1}\Big\|\,\|X^s\| \ll \Big\|b_{si-s}I + b_{si-s+1}X + \cdots + b_{si-1}X^{s-1}\Big\|.$$

Intuition: dominant terms in B_i and B_{i-1} have scalar coefficients being s indices apart from $\{b_i\}$. Consider $X = \left[\begin{smallmatrix} -1 & 1 \\ 2 & 1 \end{smallmatrix}\right]$ with $b_i = 1/i!$ and $s = 6$,

$$\|B_2\|_1 \|X^s\|_1 \approx \left\|\frac{1}{12!}I + \frac{1}{13!}X\right\|_1 \|X^s\|_1 = 6.5 \times 10^{-8}$$
$$\ll 1.8 \times 10^{-3} = \left\|\frac{1}{6!}I + \frac{1}{7!}X\right\|_1 \approx \|B_1\|_1.$$

Idea for Utilizing Multi-Precisions

$\mathrm{fl}(AB + C) = \mathrm{fl}_{high}(\mathrm{fl}_{low}(AB) + C)$ for $|A||B| \ll |C|$ and do this recursively in the evaluation of p_m.

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Exploiting Multi-Precisions in Paterson–Stockmeyer Framework

Given precisions $u_r \geq u_{r-1} \geq \cdots \geq u_v \geq u$, we compute

$$q_v(X) := \Big(\big(\big(\underbrace{\overbrace{\underbrace{\overbrace{B_r X^s}^{u_r} + B_{r-1}}_{u_{r-1}} \big) X^s}^{u_{r-1}} + B_{r-2}}_{u_{r-2}} \big) X^s + \cdots + B_v\Big) X^s$$

in the lower-than-working precisions and

$$p_m(X) = \Bigg(\Big(\big((q_v(X) + B_{v-1})X^s + B_{v-2}\big)X^s + \cdots + B_1\Big)X^s + B_0$$

in the working precision u.

Exploiting Multi-Precisions in Paterson–Stockmeyer
Error Bound

Evaluation: $$q_v(X) = \Big(\underbrace{\overbrace{\big((\underbrace{\overbrace{B_r X^s}^{u_r} + B_{r-1}}_{u_{r-1}})X^s}^{u_{r-1}} + B_{r-2}}_{u_{r-2}}\big)X^s + \cdots + B_v\Big)X^s.$$

Theorem (Error bound for $q_v(X)$)

Given $\|B_i\|\,\|X^s\| = \tau_i\,\|B_{i-1}\|$ for some $\tau_i \ll 1$, $\|\widehat{B}_i - B_i\| \le u_i\,\|B_i\|$ for $i = v\colon r$, and $\|\mathrm{fl}(X^s) - X^s\| \le u_v\,\|X^s\|$, then by setting the precisions $u_{v-1} \equiv u$ and

$$u_i = u_{i-1}/\tau_i, \quad i = v\colon r,$$

(so $u \ll u_v \ll \cdots \ll u_r$) we have

$$\|\widehat{q}_v - q_v(X)\| \lesssim (r - v + 1)nu\,\|q_v(X)\|\,,$$

where $r = \lfloor m/s \rfloor$ (assuming $((1 + \max_i \tau_i)n + 2)\,\|q_v(X)\|\,u \ll 1$).

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- If $v = 1$ and $\|\widehat{B}_0 - B_0\| \le cnu\,\|B_0\|$, $\|\widehat{p}_m - p_m(X)\| \lesssim rnu\,\|p_m(X)\|$.

[i] The required powers $X^2, \ldots, X^s$ are formed in the working precision u for the accuracy of $\widehat{B}_0$.

[ii] From standard analysis $|\,\mathrm{fl}(X^s) - X^s| \lesssim snu|X|^s$, so the condition holds if $sn\tau_v\,\|X\|^s \lesssim \|X^s\|$, or, $\|X^s\|$ not much less than $\|X\|^s$.

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Mixed-Precision Paterson–Stockmeyer

Bounds for Taylor Approximants of e^X

- For the error in $\widehat{B}_0 \approx B_0(X) = \sum_{j=0}^{s-1} b_j X^j$, standard error analysis implies

$$\left\| \widehat{B}_0 - B_0(X) \right\| \le \gamma_{(s-2)n+2} B_0(\|X\|) \approx \gamma_{(s-2)n+2} \mathrm{e}^{\|X\|}, \quad \gamma_n := \frac{nu}{1-nu},$$

then using $1 \le \left\|\mathrm{e}^X\right\| \left\|\mathrm{e}^{-X}\right\| \le \left\|\mathrm{e}^X\right\| \mathrm{e}^{\|X\|}$,

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- A sufficient condition for $\|\mathrm{fl}(X^s) - X^s\| \le u_v \|X^s\|$ is $sn\tau_v \|X\|^s \lesssim \|X^s\|$, one can show

$$\frac{sn\tau_v \|X\|_1^s}{\|X^s\|_1} = \frac{sn\|B_v\|_1 \|X\|_1^s}{\|B_{v-1}\|_1} \lesssim \begin{cases} sn\mathrm{e}^{\|X\|_1}, & v = 1, \\ sn/\binom{vs}{s}, & v > 1, \end{cases}$$

with the asumption $\|X\|_1 \le s/\mathrm{e}$.

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Mixed-Precision Paterson–Stockmeyer

The General Algorithm

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Input   : $X \in \mathbb{C}^{n\times n}$, $\{b_i\}_{i=0}^{m} \subset \mathbb{C}$
Output: $P \approx p_m(X)$
$s \leftarrow \lceil \sqrt{m} \rceil,\ r \leftarrow \lfloor m/s \rfloor,\ v \leftarrow r+1$
Compute $\mathcal{X} := \{X^i\}_{i=2}^{s}$ and $B_0$ in precision $u \equiv u_0$
for $i \leftarrow 1$ to $r$ do
    Assemble $B_i$ using elements in $\mathcal{X} \cup \{I, X\}$ and estimate $\|B_i\|_1$
    $u_i \leftarrow \|B_{i-1}\|_1 u_{i-1} / (\|B_i\|_1 \|X^s\|_1)$        ▷ $u_i = u_{i-1}/\tau_i,\ \tau_i \ll 1$
$v \leftarrow \min\{i \colon u_i \geq \delta u\},\ u_{v-1}, u_{v-2}, \dots, u_1 \leftarrow u,\ P \leftarrow B_r$
for $i \leftarrow r$ down to $1$ do
    Compute $P \leftarrow PX^s$ in precision $u_i$
    Form $P \leftarrow P + B_{i-1}$ in precision $u_{i-1}$
return $P$
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- need store $\{X^i\}_{i=1}^{s}$ and $\{B^i\}_{i=0}^{r}$: about $2sn^2$ elements of storage
- $s+v-2$ matrix products in u and 1 in each of $u_v, u_{v+1}, \dots, u_r$.

- How practical is the algorithm (are the conditions $\tau_i \ll 1$, $i = v \colon r$)?

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Theorem (Decay of τ_i)

If $\|X\|_1 \le s/\mathrm{e}$, for $i = 2\colon r$,

$$\tau_i = \frac{\|B_i\|_1 \|X^s\|_1}{\|B_{i-1}\|_1} \lesssim \frac{\mathrm{e}}{\mathrm{e}-1} i^{-s} \approx 1.58 i^{-s}.$$

- τ_i decreases at least polynomially as i increases and at least exponentially as s increases.
- Bound not applicable to τ_1 $\Rightarrow$ we have the bound

$$\tau_1 = \frac{\|B_1\|_1 \|X^s\|_1}{\|B_0\|_1} \lesssim \frac{\|X\|_1^s}{s!\|B_0\|_1} \cdot \frac{\|X^s\|_1}{\|X\|_1^s} \lesssim \frac{1}{\|\mathrm{e}^X\|_1} \cdot \frac{\|X^s\|_1}{\|X\|_1^s} \le 1.$$

- A special treatment for $\|X\|_1 \le s/\mathrm{e}$ is possible: choose s sufficiently large s.t. $\tau_i \ll 1$, $i = 1\colon r$.
- Insight for the general case (?): larger s makes v in $\tau_i \ll 1$, $i = v\colon r$ smaller. (Recall $s+v-2$ matrix products in u and 1 in $u_v, u_{v+1}, \dots, u_r$).

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- τ_i decreases at least polynomially as i increases and at least exponentially as s increases.
- Bound not applicable to τ_1 $\Rightarrow$ we have the bound

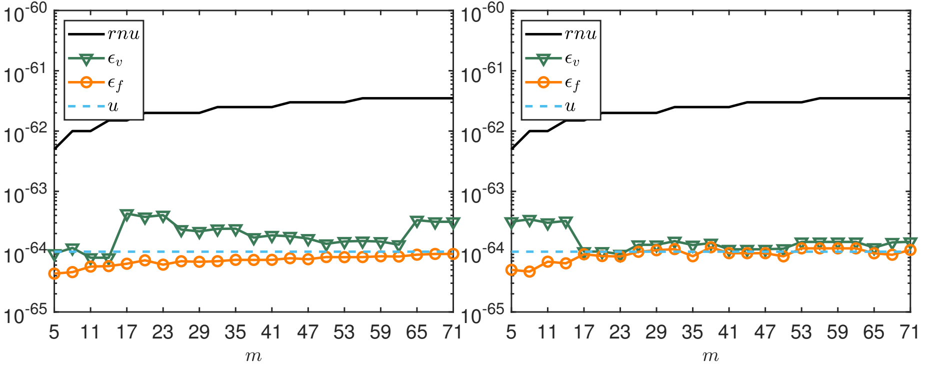
$$\tau_1 = \frac{\|B_1\|_1 \|X^s\|_1}{\|B_0\|_1} \lesssim \frac{\|X\|_1^s}{s!\|B_0\|_1} \cdot \frac{\|X^s\|_1}{\|X\|_1^s} \lesssim \frac{1}{\|\mathrm{e}^X\|_1} \cdot \frac{\|X^s\|_1}{\|X\|_1^s} \le 1.$$

• A special treatment for $\|X\|_1 \le s/\mathrm{e}$ is possible: choose s sufficiently large s.t. $\tau_i \ll 1$, $i = 1\colon r$.

• Insight for the general case (?): larger s makes v in $\tau_i \ll 1$, $i = v\colon r$ smaller. (Recall $s + v - 2$ matrix products in u and 1 in $u_v, u_{v+1}, \dots, u_r$).

Numerical Experiments

p_m from Taylor Approximant of $\exp$, Varying m



Left: $X = \texttt{rand(n)}$. Right: $X = \texttt{randn(n)}$. $n = 50$.

$\|X\|_1 = \lceil\sqrt{m}\rceil/\mathrm{e}$, Variable-precision environment with $u = 10^{-64}$ (Simulated by **Advanpix**), and $\epsilon = \|\widehat{p}_m - p_m(X)\|_1/\|p_m(X)\|_1$.

Numerical Experiments

Complexity Reduction in Variable Precisions

Table: m: minimal degree such that $\|e^X - p_m(X)\|_1 \le u$. d_i: equivalent decimal digits of precision u_i. C_p: approximate complexity reduction in percentage (assuming complexity is linearly proportional to the number of digits used).

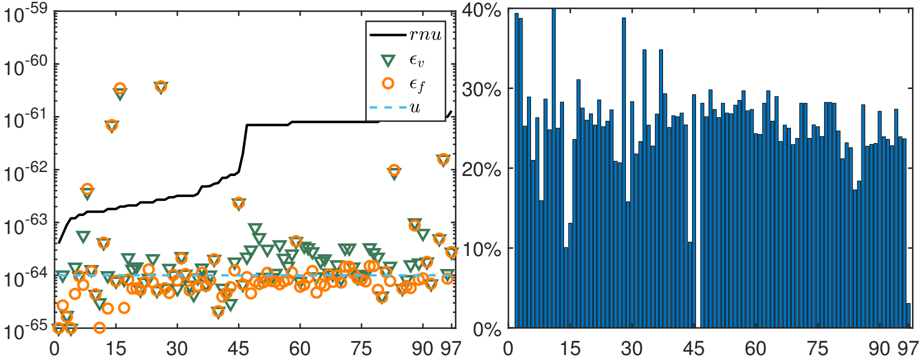
(u, m)	(s, r)	$(d_1, d_2, \ldots, d_r)$	C_p
$(10^{-32}, 37)$	$(7, 5)$	$(30, 25, 18, 11, 3)$	20.7%
$(10^{-64}, 60)$	$(8, 7)$	$(61, 55, 47, 38, 28, 18, 7)$	21.6%
$(10^{-128}, 99)$	$(10, 9)$	$(124, 115, 104, 92, 78, 64, 49, 34, 18)$	20.6%
$(10^{-256}, 169)$	$(13, 13)$	$(249, 237, 221, 203, 184, 164, 143, 121, 99, 75, 52, 28, 3)$	24.2%

$X =$ `gallery('cauchy',n)` for $n = 100$ with $\|X\|_1 \approx 4.20$

- $\tau_i = u_{i-1}/u_i = 10^{d_i - d_{i-1}}$ is in general decreasing (w.r.t. i), 20% of the matrix products were performed in precision $u^{1/2}$ or much lower.

Numerical Experiments

p_m from Taylor Approximant of $\exp$, $u = 10^{-64}$

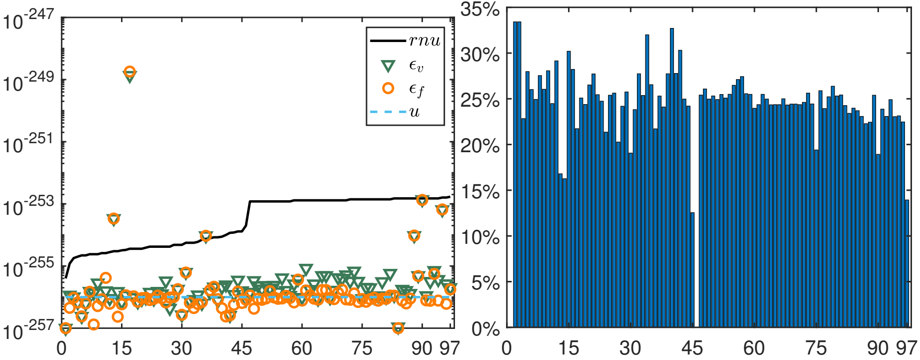


97 non-Hermitian matrices from **(Fasi and Higham, 2018)**, $2 \leq n \leq 100$. The degree m and scaling ℓ are from $\mathrm{e}^A \equiv \mathrm{e}^{2^\ell X} \approx p_m(X)^{2^\ell}$. $u = 10^{-64}$.

Left: $\epsilon = \|\widehat{p}_m - p_m(X)\|_1 / \|p_m(X)\|_1$. Right: the approximate percentages of complexity reduction.

Numerical Experiments

p_m from Taylor Approximant of $\exp$, $u = 10^{-256}$

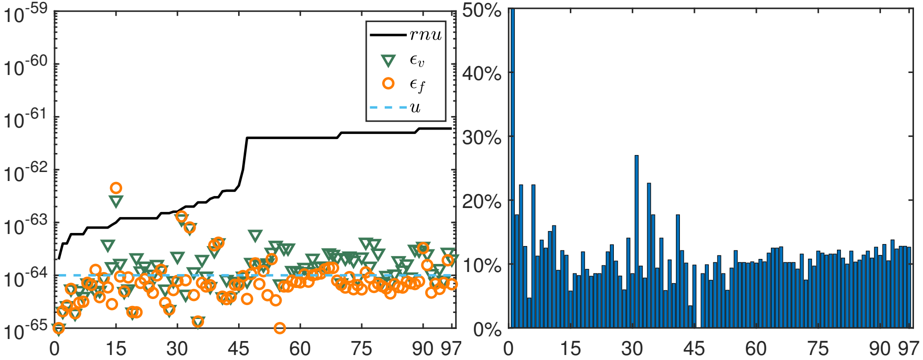


97 non-Hermitian matrices from **(Fasi and Higham, 2018)**, $2 \le n \le 100$. The degree m and scaling ℓ are from $\mathrm{e}^{A} \equiv \mathrm{e}^{2^{\ell}X} \approx p_m(X)^{2^{\ell}}$. $u = 10^{-256}$.

Left: $\epsilon = \|\widehat{p}_m - p_m(X)\|_1 / \|p_m(X)\|_1$. Right: the approximate percentages of complexity reduction.

Numerical Experiments

p_m from Padé Approximant of $\exp$ (Numerator)

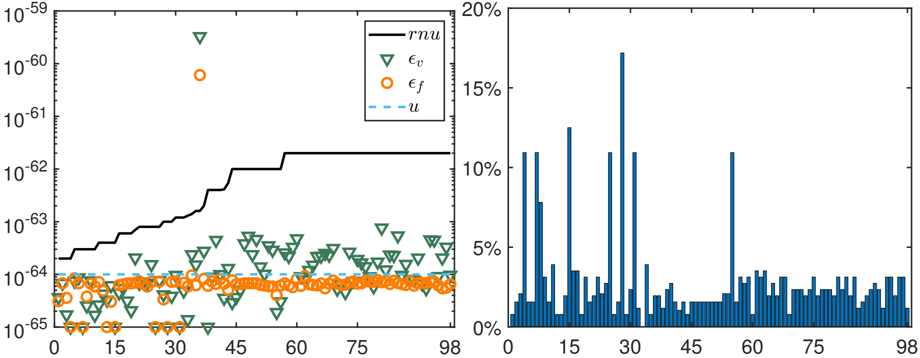


97 non-Hermitian matrices from **(Fasi and Higham, 2018)**, $2 \leq n \leq 100$. The degree m and scaling ℓ are from $\mathrm{e}^{A} \equiv \mathrm{e}^{2^{\ell}X} \approx r_{mm}(X)^{2^{\ell}}$. $u = 10^{-64}$.

- Scalar coefficients from Padé decay faster than from Taylor and smaller degree m is chosen!

Numerical Experiments

p_m from Taylor Approximant of $\cos$



98 non-Hermitian matrices from **(Al-Mohy, Higham and L, 2022)**, $4 \le n \le 100$. The degree m and scaling ℓ are from $\mathrm{e}^A \equiv \mathrm{e}^{2^\ell X} \approx p_m(X)^{2^\ell}$. $u = 10^{-64}$.

- Scalar coefficients for $\cos$ decay faster than for $\exp$ and smaller degree m is chosen (plus $p_m(X^2)$ is actually evaluated via Paterson–Stockmeyer).

Conclusions

- Lower(-than-working) precisions can be exploited in the Paterson–Stockmeyer method, if $\|X\|$ is “small” (which (I think) is satisfied in most of the practical cases) and modulus of the scalar coefficients decays quickly.
- The key idea is to perform computations on data of small magnitude (norm) in low precision.
- Better understanding of the method is desired (e.g., for $\exp$ the algorithm works well and the bound appears pessimistic).

▶ X. Liu. Mixed-precision Paterson–Stockmeyer method for evaluating polynomials of matrices. preprint, https://arxiv.org/abs/2312.17396.

Thank you for your attention!

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