Mixed-precision Paterson–Stockmeyer Method for Evaluating Matrix Polynomials

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10th International Congress on Industrial and Applied Mathematics, Waseda University, Tokyo, August 22, 2023

Matrix Polynomials

We want to evaluate the matrix polynomial

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

where

- $m \in \mathbb{N}$,
- $b_i \in \mathbb{C}$ and mostly nonzero,
- $X \in \mathbb{C}^{n \times n}$.

Motivation

- Computation of matrix functions
  - series expansion (Taylor series)
  - rational functions $q(X)^{-1}p(X)$
- Solution of matrix equations

Paterson–Stockmeyer Method

For a positive integer s, we can rewrite **(Paterson and Stockmeyer, 1973)**

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

where

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

- $p_m(X)$ is a polyn. in X^s with coefficients B_i: e.g., $(s = 3)$,

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

Paterson–Stockmeyer Method: Evaluation

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

Input : $X \in \mathbb{C}^{n\times n}$, $b_0, b_1, \ldots, b_m \in \mathbb{C}$

Output: $Z = p_m(X)$

$\mathcal{X}_0 \leftarrow I$, $\mathcal{X}_1 \leftarrow X$

for $i \leftarrow 2$ **to** s **do**

  $\mathcal{X}_i \leftarrow X \mathcal{X}_{i-1}$ ▷ *$X^2, \ldots, X^s$ computed and stored*

end

$Z \leftarrow \sum_{j=0}^{m-sr} b_{sr+j} \mathcal{X}_j$

for $i \leftarrow r - 1$ **down to** 0 **do**

  $Z \leftarrow Z \mathcal{X}_s + \sum_{j=0}^{s-1} b_{si+j} \mathcal{X}_j$

end

return Z

Paterson–Stockmeyer (PS) Method

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

- $(s-1)n^2$ additional storage
- about $s + r - 1$ matrix products (recall that $r = \lfloor m/s \rfloor$)

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 Mutiple Precisions in PS

Practical considerations:

- $\|X\|$ **is usually small**;
- b_i **can decay quickly**, e.g., the Taylor series of exp, cos.

For PS method

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

can we have $\|B_i\| \, \|X^s\| \ll \|B_{i-1}\|$, $i = r : 1$?

Key idea: 1. If $|A| \le |C|, |B| \le |C|$, and $|A||B| \ll |C|$, computing the product in $AB + C$ in a lower precision than the addition:

$$\mathrm{fl}_{high}(\mathrm{fl}_{low}(AB) + C).$$

2. Apply the above idea recursively in the evaluation of p_m.

Exploiting Multi-Precisions in PS: Framework

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

$$\underbrace{(\underbrace{B_r X^s + B_{r-1}}_{u_{r-1}}) X^s + B_{r-2}}_{u_{r-2}}$$

where we require

$$\|\widehat{B}_i - B_i\| \le u_i \|B_i\|, \ i = r:0, \quad \|\widehat{X^s} - X^s\| \le u_1 \|X^s\|,$$

and the precisions u_i are chosen by

$$u_i = \frac{\|B_0\|}{\|B_i\| \, \|X^s\|^i} u_0, \quad i = 1:r,$$

which means $u = u_0 \ll u_1 \ll \cdots \ll u_r$ since

$$\frac{u_i}{u_{i-1}} = \frac{\|B_{i-1}\|}{\|B_i\| \, \|X^s\|} \gg 1, \quad i = 1:r.$$

Exploiting Multi-Precisions in PS: Framework

If $\|B_i\| \, \|X^s\| \le \tau \, \|B_{i-1}\|$, $i = r\colon 1$ for some $\tau \ll 1$ (by choosing a suitable s), we then have **(Higham and L, Working note)**

$$\|\widehat{p}_m - p_m(X)\| \lesssim rnu \, \|p_m(X)\| \,,$$

where $r = \lfloor m/s \rfloor$.

• Do we have $\|\widehat{B}_i - B_i\| \le u_i \, \|B_i\| \,, \; i = r\colon 0$ and $\|\widehat{X^s} - X^s\| \le u_1 \, \|X^s\|$?

1. Form $\mathcal{X} = \{X^2, X^3, \dots, X^s\}$ in u_0 (note $u_0 \ll u_1$).

2. Compute B_i using the powers in $\mathcal{X}$ and downgrade B_i to u_i (after estimating $\|B_i\|$).

Question: Is it possible to use u_0 and a lower precision $u_\ell > u_0$ in forming the powers in $\mathcal{X}$?

Explicit Powering for B_0 Using Two Precisions

Key idea: For the matrix sum $X_1 + X_2$ in u_h (in our case $u_h = u_0$), where $\|X_2\| \ll \|X_1\|$. X_2 can be stored in a lower precision

$$u_\ell \le \frac{u_h \|X_1 + X_2\|}{(1+u_h)\|X_2\|} \approx \frac{u_h \|X_1\|}{\|X_2\|}.$$

$\widetilde{X}_2$: X_2 converted into precision $u_\ell > u_h$, we have

$$\mathrm{fl}_h(X_1 + \widetilde{X}_2) = (X_1 + X_2(1+\delta_\ell))(1+\delta_h), \ |\delta_h| \le u_h, \ |\delta_\ell| \le u_\ell,$$

and

$$E := \mathrm{fl}_h(X_1 + \widetilde{X}_2) - (X_1 + X_2) = \delta_h(X_1 + X_2) + \delta_\ell(1+\delta_h)X_2$$

with

$$\|E\| \le u_h \|X_1 + X_2\| + u_\ell(1+u_h)\|X_2\| \le 2u_h \|X_1 + X_2\|.$$

Explicit Powering for B_0 Using Two Precisions

Track the norm of $\mathrm{fl}_h(q_j(X)) := \mathrm{fl}_h(b_0 I + b_1 X + \cdots + b_j X^j)$, until, for $j = t$,

$$\frac{u_\ell}{u_h} \lesssim \frac{\|q_t(X)\|}{|b_{t+1}| \, \|X^{t_1}\| \, \|X^{t_2}\|} \Rightarrow \frac{u_\ell}{u_h} \lesssim \frac{\|q_t(X)\|}{\|b_{t+1} X^{t+1}\|} \approx \frac{\|\mathrm{fl}_h(q_t(X))\|}{\|b_{t+1} X^{t+1}\|},$$

where $t_1 + t_2 = t + 1$.

- Can find the best available t_1, t_2 in t norm estimations.

If $\left\|b_{t+2} X^{t+2}\right\| \lesssim \left\|b_{t+1} X^{t+1}\right\|$, next,

$$\frac{\left\|q_t(X) + b_{t+1} X^{t+1}\right\|}{\left\|b_{t+2} X^{t+2}\right\|} \gtrsim \frac{\|q_t(X)\| - \left\|b_{t+1} X^{t+1}\right\|}{\left\|b_{t+2} X^{t+2}\right\|} \gtrsim \frac{u_\ell}{u_h} - 1 \approx \frac{u_\ell}{u_h}.$$

- Can form the rest of the required powers $X^{t+1}, \ldots, X^{s-1}$ in precision $u_\ell > u_h$, if

$$\left\|b_{t+1} X^{t+1}\right\| \gtrsim \left\|b_{t+2} X^{t+2}\right\| \gtrsim \cdots \gtrsim \left\|b_{s-1} X^{s-1}\right\|.$$

Taylor Approximant of the Matrix Exponential

Theorem 1.

If $\|X\|_1 \le \sqrt[s]{s!}(\approx s/\mathrm{e}+1)$, for $i = 2\colon r$ and sufficiently large $s \ge 3$,

$$\frac{\|B_{i-1}\|_1}{\|B_i\|_1 \|X^s\|_1} \gtrsim \left(1 - \frac{1}{\mathrm{e}i}\right) i^s.$$

Recall that we need to choose s such that $\|B_i\| \, \|X^s\| \le \tau \, \|B_{i-1}\|$, $i = r\colon 1$ **for some** $\tau \ll 1$ in computing

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

- For a fixed $s \ge 3$, the ratio $\|B_{i-1}\|_1/(\|B_i\|_1 \|X^s\|_1)$ tends to increase polynomially as i increases, $i = 2\colon r$.

- Bound not applicable for $\|B_0\|_1/(\|B_1\|_1 \|X^s\|_1)$.

For the Matrix Exponential: the Algorithm

Input : $X \in \mathbb{C}^{n\times n}$, $m \in \mathbb{N}^+$, $u > 0$
Output: A Taylor approximant P of order m for e^X

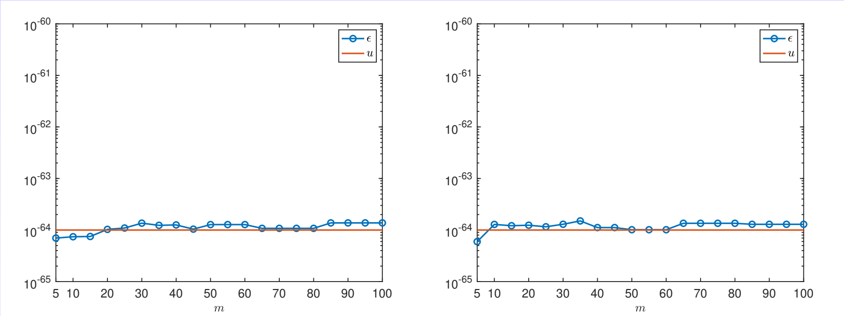
$s \leftarrow \lceil \sqrt{m} \rceil$, $u_0 \leftarrow u$, $\mathcal{X}_0 \leftarrow I$, $\mathcal{X}_1 \leftarrow X$
Compute B_0 and $Y = X^s$ in u (and potentially $u_\ell > u$)
while $(\mathrm{e}-1)s!\|B_0\|_1 \le \mathrm{e}\tau\|Y\|_1$ **and** $s < m$ **do**
    $B_0 \leftarrow B_0 + Y/s!$, $s \leftarrow s+1$
    Update $\mathcal{X}_s \leftarrow XY$ and $Y \leftarrow \mathcal{X}_s$
end
for $i \leftarrow 1$ **to** $r \leftarrow \lfloor m/s \rfloor$ **do**
    Compute B_i using elements in $\mathcal{X}$ and estimate $\|B_i\|_1$
    Downgrade B_i to $u_i \leftarrow u_{i-1}\|B_{i-1}\|_1/(\|B_i\|_1\|Y\|_1)$
end
$P = B_r$
for $i \leftarrow r$ **to** 1 **do**
    Convert Y into u_i and compute $P \leftarrow PY$ in u_i
    Form $P \leftarrow P + B_{i-1}$ in u_{i-1}
end
return P

The Parameter s and the Cost

- The matrix products in computing B_0 are most expensive: smaller s with larger $r = \lfloor m/s \rfloor$ benefits efficiency
- Smaller s puts a more strict requirement: $\|X\|_1 \le \sqrt[s]{s!}$
- A larger s is more likely to be accepted by the algorithm

Overall cost: $\lceil \sqrt{m} \rceil - 1 \le s - 1 \le m - 1$ matrix multiplications in precision u and 1 matrix multiplication in each of $u_i > u$, $i = 1\colon r$, where $1 \le r = \lfloor m/s \rfloor \le \lceil \sqrt{m} \rceil$.

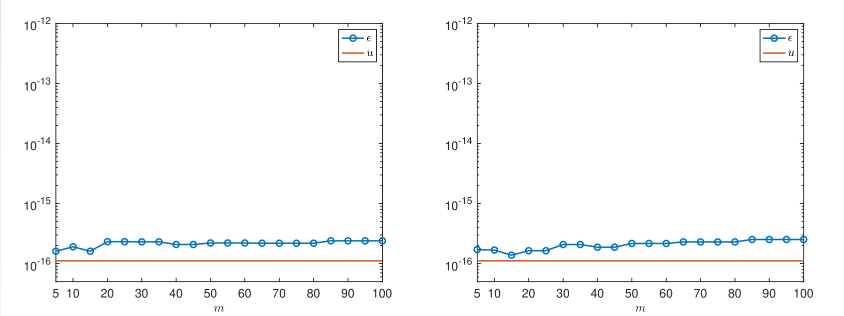
Numerical Experiment Using High Precisions



Left: $X =$ `rand(n)`. Right: $X =$ `randn(n)`. $n = 50$

$\|X\|_1 = 1$, $u = 10^{-64}$ (Simulated by **Advanpix Multiprecision Computing Toolbox**), and $\epsilon = \left\|\widehat{p}_m - p_m(X)\right\| / \|p_m(X)\|$.

Numerical Experiment Using Low Precisions



Left: $X =$ `rand(n)`. Right: $X =$ `randn(n)`. $n = 50$

$\|X\|_1 = 1$, $u = 2^{-53} \approx 1.1 \times 10^{-16}$, and
$\epsilon = \left\|\widehat{p}_m - p_m(X)\right\| / \|p_m(X)\|$.

- Only double, single, and half (simulated by `chop`) **(Higham and Pranesh, 2019)** precisions are used.

Numerical Experiment: Approximating $\exp(X)$

Table: The minimal degree m such that the error in approximating the matrix exponential via a Taylor approximant is of order u. d_i represents the equivalent decimal digits of precision u_i.

(u, m)	(s, r)	$(d_1, d_2, \ldots, d_r)$
$(10^{-32}, 32)$	$(6, 5)$	$(30, 26, 20, 13, 6)$
$(10^{-64}, 54)$	$(8, 6)$	$(61, 54, 45, 35, 24, 13)$
$(10^{-128}, 92)$	$(10, 9)$	$(123, 113, 101, 88, 73, 58, 42, 25, 8)$
$(10^{-256}, 158)$	$(13, 12)$	$(248, 234, 217, 198, 178, 156, 133, 110, 86, 62, 36, 11)$

$X =$ `gallery('cauchy',n)` for $n = 20$ with $\|X\|_1 \approx 2.65$

- The default $s = \lceil \sqrt{m} \rceil$ is chosen in all cases, and 20% of the matrix products were performed in precision $u^{1/2}$ or much lower.

Concluding Remarks

- Lower precisions can be used in the PS method if $\|X\|$ is small and the coefficients decay quickly.

- The key idea is to perform computations on data of small magnitude (norm) in low precision.

N. J. Higham and X. Liu. Mixed-precision Paterson–Stockmeyer method for evaluating matrix polynomials. Working note.

Proof of Thm. 1: I

We have, with $\|X\|_1 =: \sigma \le \sqrt[s]{s!}$, for $i = 2\colon r$ and $s \ge 3$,

$$\frac{\|B_{i-1}\|_1}{\|B_i\|_1\|Y\|_1} = \frac{\left\| \frac{1}{((i-1)s)!}I + \frac{1}{((i-1)s+1)!}X + \cdots + \frac{1}{((i-1)s+s-1)!}X^{s-1} \right\|_1}{\left\| \frac{1}{(is)!}I + \frac{1}{(is+1)!}X + \cdots + \frac{1}{(is+s-1)!}X^{s-1} \right\|_1 \|X^s\|_1}$$

$$\ge \frac{\frac{1}{((i-1)s)!} - \left(\frac{\sigma}{((i-1)s+1)!} + \frac{\sigma^2}{((i-1)s+2)!} + \cdots + \frac{\sigma^{s-1}}{((i-1)s+s-1)!} \right)}{\left(\frac{1}{(is)!} + \frac{\sigma}{(is+1)!} + \cdots + \frac{\sigma^{s-1}}{(is+s-1)!} \right) s!}$$

$$\ge \frac{\frac{1}{((i-1)s)!} - \frac{\sigma}{((i-1)s+1)!} \left(1 + \frac{\sigma}{(i-1)s+2} + \cdots + \frac{\sigma^{s-2}}{((i-1)s+2)^{s-2}} \right)}{\frac{1}{(is)!} \left(1 + \frac{\sigma}{is+1} + \cdots + \frac{\sigma^{s-1}}{(is+1)^{s-1}} \right) s!}$$

$$=: \gamma(s).$$

Proof of Thm. 1: II

On the other hand, we know from Stirling's approximation

$$\frac{\sigma}{s} \leq \frac{\sqrt[s]{s!}}{s} \sim \frac{\sqrt[2s]{2\pi s}}{\mathrm{e}} \to \mathrm{e}^{-1}, \quad s \to \infty,$$

which says σ grows at most (linearly) like $\mathrm{e}^{-1}s$ for sufficiently large s. Therefore, we have, for sufficiently large s,

$$\gamma(s) = \frac{\frac{1}{((i-1)s)!} - \frac{\sigma}{((i-1)s+1)!} \cdot \frac{1-(\sigma/((i-1)s+2))^{s-1}}{1-\sigma/((i-1)s+2)}}{\frac{s!}{(is)!} \cdot \frac{1-(\sigma/(is+1))^{s}}{1-\sigma/(is+1)}} \sim \frac{(is)!\left(1 - \frac{\sigma}{is+1}\right)}{s!(is-s)!}$$

$$\gtrsim \left(1 - \frac{1}{\mathrm{e}i}\right)\binom{is}{s} \geq \left(1 - \frac{1}{\mathrm{e}i}\right)\frac{(is)^s}{s^s} = \left(1 - \frac{1}{\mathrm{e}i}\right)i^s. \qquad \square$$

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