Fast computation of exp(Toeplitz)

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Aim

Given an $n \times n$ Toeplitz matrix

$$T = \begin{bmatrix} t_0 & t_{-1} & \cdots & t_{-n+1} \\ t_1 & t_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & t_{-1} \\ t_{n-1} & \cdots & t_1 & t_0 \end{bmatrix},$$

compute $\exp(T)$ in less than $O(n^3)$ operations.

Motivation

- Discretization of partial integro-differential equations (PIDEs) with a shift-invariant kernel.
- Pricing of single-asset options modelled by jump-diffusion processes.

Example: Merton model requires solution of PIDE

$$\omega_t = \frac{\nu^2}{2}\omega_{\xi\xi} + \left(r - \lambda\kappa - \frac{\nu^2}{2}\right)\omega_\xi - (r+\lambda)\omega + \lambda\int_{-\infty}^{\infty}\omega(\xi+\eta, t)\phi(\eta)d\eta$$

on domain $(\xi, t) \in (-\infty, \infty) \times [0, t_e]$.

Truncation of $(-\infty, \infty)$ and discretization by standard finite differences/rectangle rule $\rightsquigarrow$

$$w(t+h) = \exp(hT)w_t.$$

Explicit availability of $\exp(hT)$ useful for computing (many) prices at fixed time intervals (e.g., for every day).

Selected related work

If T is (block-)triangular (block-)Toeplitz then $\exp(T)$ inherits this structure:

D. A. Bini, S. Dendievel, G. Latouche, and B. Meini, Computing the exponential of large block-triangular block-Toeplitz matrices encountered in fluid queues, arXiv:1502.07533, 2015.

Fast Toeplitz solvers combined with rational Arnoldi for computing $\exp(T)b$:

S. T. Lee, H.-K. Pang, and H.-W. Sun, Shift-invert Arnoldi approximation to the Toeplitz matrix exponential, SIAM J. Sci. Comput., 32 (2010), pp. 774–792,

Outline

Displacement rank

Displacement rank

Consider displacement

$$\nabla(A) = A - ZAZ^*, \qquad Z = \begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{bmatrix}.$$

For $A =$ Toeplitz:

$$\nabla(T) = T - ZTZ^* = \begin{bmatrix} t_0 & t_{-1} & \cdots & t_{-n+1} \\ t_1 & 0 & \ddots & 0 \\ \vdots & 0 & \ddots & \vdots \\ t_{n-1} & 0 & \cdots & 0 \end{bmatrix},$$

Toeplitz matrix T has rank$(\nabla(T))$ at most 2.

Reconstruction from displacement

$$A - ZAZ^* = GB^*$$

with $B, G \in \mathbb{C}^{n\times r}$ is matrix Stein equation with unique solution

$$\begin{aligned} A = \mathcal{T}(G,B) \quad &:= \quad \sum_{k=0}^{n-1} Z^k GB^*(Z^*)^k \\ &= \quad L(g_1)U(b_1^*) + L(g_2)U(b_2^*) + \cdots + L(g_r)U(b_r^*), \end{aligned}$$

where

$$L(x) := \begin{bmatrix} x_1 & 0 & \cdots & 0 \\ x_2 & x_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ x_n & \cdots & x_2 & x_1 \end{bmatrix}, \qquad U(x) := \begin{bmatrix} x_1 & x_2 & \cdots & x_n \\ 0 & x_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & x_2 \\ 0 & \cdots & 0 & x_1 \end{bmatrix}.$$

$\rightsquigarrow$ Exact and fast reconstruction of matrix from its generator (G, B).

T^{-1} has displacement rank ≤ 2

Well-known results:

- Inverse of Toeplitz matrix T has displacement rank ≤ 2.
- General matrix A: $\text{rank}(\nabla(A^{-1})) \leq \text{rank}(\nabla(A)) + 2$

Proof based on embedding into larger matrix of low displacement rank and utilizing that Schur complements preserve displacement ranks.

Selected references:

- T. Kailath and A. Sayed, *Displacement structure: theory and applications*, SIAM Review, 37 (1995), pp. 297–386.
- T. Kailath and A. H. Sayed, *Fast Reliable Algorithms for Matrices with Structure*, SIAM, Philadelphia, 1999.
- V. Olshevsky, ed., *Structured matrices in mathematics, computer science, and engineering. I*, vol. 280 of Contemporary Mathematics, American Mathematical Society, Providence, RI, 2001.

expm(T) does not have low displacement rank

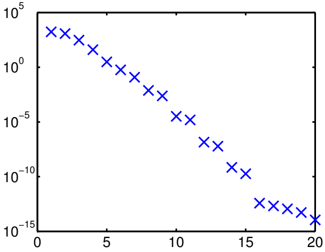
```
>> n = 20; A = toeplitz(randn(n,1));
>> Z = [zeros(1,n); eye(n-1,n) ];
>> rank(A-Z*A*Z'),
ans =
     2
```

expm(T) does not have low displacement rank

```
>> n = 20; A = toeplitz(randn(n,1));
>> Z = [zeros(1,n); eye(n-1,n) ];
>> rank(A-Z*A*Z'),
ans =
     2
>> rank(expm(A)-Z*expm(A)*Z'),
ans =
    15
```

expm(T) often has low *approximate* displacement rank

```
>> n = 20; A = toeplitz(randn(n,1));
>> Z = [zeros(1,n); eye(n-1,n) ];
>> rank(A-Z*A*Z'),
ans =
     2
>> rank(expm(A)-Z*expm(A)*Z'),
ans =
    15
>> svd(expm(A)-Z*expm(A)*Z'),
```



Approximate displacement rank

Stability of generator

Lemma. [Pan'1993, DK/Luce'2016] Displacement $\nabla(A)$ for $A \in \mathbb{C}^{n\times n}$ satisfies

$$\frac{1}{2}\|\nabla(A)\|_* \leq \|A\|_* \leq n\|\nabla(A)\|_*,$$

for any unitarily invariant norm $\|\cdot\|_*$.

Consequences:

- By linearity of ∇:
  $\frac{1}{2}\|\nabla(A) - \nabla(\tilde{A})\|_* \leq \|A - \tilde{A}\|_* \leq n\|\nabla(A) - \nabla(\tilde{A})\|_*$.
- Low-rank truncation of generator $\Leftrightarrow$ approximation of matrix.

A priori result by rational approximation

Theorem. [DK/Luce'2016] Let T Toeplitz, p, q polynomials. Then $r(T) = p(T)[q(T)]^{-1}$ has displacement rank at most

$$2 \max\{\deg p, \deg q\} + 1.$$

Theorem. [Gonchar/Rakhmanov'1987] $\exists$ constant C such that

$$\inf_{p_1, p_2 \in \mathcal{P}_s} \max_{\lambda \in (-\infty, 0]} |e^{\lambda} - p_1(\lambda)/p_2(\lambda)| \leq C\, V^{-s}$$

holds for all $s \geq 1$ with $V \approx 9.28903\ldots$.

Corollary. Let T be symmetric negative definite. Then

$$\min\{\|\exp(T) - A\|_2 : \operatorname{rank}(\nabla(A)) \leq 2s + 1\} \leq C\, V^{-s}.$$

- Technique extends to other rational approximation results (e.g., [López-Fernández/Palencia/Schädle'2006] for sectoral operators).

Scaling & Squaring

Scaling & Squaring

Basic idea:

1. Scale $\tilde{A} = 2^{-\rho} A$, $\rho \geq 0$, s.t. $\|\tilde{A}\| \lesssim 1$.
2. Compute (low-degree) rational approximation $\tilde{E} = p(\tilde{A}) q(\tilde{A})^{-1} \approx \exp(\tilde{A})$.
3. Compute $E = \tilde{E}^{2^\rho}$ by squaring ρ times.

Remarks:

- No properties on A known: choose diagonal Padé approximation p/q.
  Basis of MATLAB's `expm`, [Higham'2008], [Higham'2009], ...
- Eigenvalues of A on or very close to negative real axis: choose subdiagonal Padé approximation p/q.
  Basis of `sexpm` by [Güttel/Nakatsukasa'2016].

Scaling & Squaring

Input: General matrix $A \in \mathbb{C}^{n \times n}$.

Output: Accurate approximation $E \approx \exp(A)$.

Compute $\|A\|_1$

Choose scaling parameter ρ and Padé approximant $r_m(z) = \frac{p_m(z)}{q_m(z)}$

Scale $A \leftarrow 2^{-\rho} A$.

Compute $U \leftarrow p_m(A)$, $V \leftarrow q_m(A)$.

Compute $E \leftarrow UV^{-1}$.

for $k = 1$ **to** ρ **do**

  $E \leftarrow E \cdot E$.

end for

Scaling & Squaring for Toeplitz matrices

Input: Toeplitz matrix $T \in \mathbb{C}^{n \times n}$.
Output: Accurate approximation $E \approx \exp(T)$.

Compute $\|T\|_1$
Choose scaling parameter ρ and Padé approximant $r_m(z) = \frac{p_m(z)}{q_m(z)}$
Scale $T \leftarrow 2^{-\rho} T$.
Compute $U \leftarrow p_m(T)$, $V \leftarrow q_m(T)$.
Compute $E \leftarrow UV^{-1}$.
for $k = 1$ **to** ρ **do**
    $E \leftarrow E \cdot E$.
end for

Scaling & Squaring for Toeplitz matrices

Input: Toeplitz matrix $T \in \mathbb{C}^{n \times n}$.

Output: Accurate approximation $E \approx \exp(T)$.

Compute $\|T\|_1$ $\{\mathcal{O}(n)\}$
Choose scaling parameter ρ and Padé approximant $r_m(z) = \frac{p_m(z)}{q_m(z)}$
Scale $T \leftarrow 2^{-\rho} T$.
Compute $U \leftarrow p_m(T)$, $V \leftarrow q_m(T)$.
Compute $E \leftarrow UV^{-1}$.
for $k = 1$ **to** ρ **do**
    $E \leftarrow E \cdot E$.
end for

Remark:

- Simple to see that $\|T\|_1$ can be computed in $\mathcal{O}(n)$ operations.

Scaling & Squaring for Toeplitz matrices

Input: Toeplitz matrix $T \in \mathbb{C}^{n \times n}$.

Output: Accurate approximation $E \approx \exp(T)$.

Compute $\|T\|_1$ $\{\mathcal{O}(n)\}$

Choose scaling parameter ρ and Padé approximant $r_m(z) = \frac{p_m(z)}{q_m(z)}$

Scale $T \leftarrow 2^{-\rho} T$. $\{\mathcal{O}(n)\}$

Compute $U \leftarrow p_m(T)$, $V \leftarrow q_m(T)$.

Compute $E \leftarrow UV^{-1}$.

for $k = 1$ **to** ρ **do**

  $E \leftarrow E \cdot E$.

end for

Remark:

- Rescale only first column and row of T.

Scaling & Squaring for Toeplitz matrices

Input: Toeplitz matrix $T \in \mathbb{C}^{n \times n}$.

Output: Accurate approximation $E \approx \exp(T)$.

```
Compute ‖T‖₁                                                {O(n)}
Choose scaling parameter ρ and Padé approximant r_m(z) = p_m(z)/q_m(z)
Scale T ← 2^{-ρ} T.                                         {O(n)}
(G_p, B_p) ← generator for p_m(T)                           {O(mn log n)}
(G_q, B_q) ← generator for q_m(T)                           {O(mn log n)}
Compute E ← U V^{-1}.
for k = 1 to ρ do
    E ← E · E.
end for
```

- Compute $\|T\|_1$ $\quad\{\mathcal{O}(n)\}$
- Choose scaling parameter ρ and Padé approximant $r_m(z) = \frac{p_m(z)}{q_m(z)}$
- Scale $T \leftarrow 2^{-\rho} T$. $\quad\{\mathcal{O}(n)\}$
- $(G_p, B_p) \leftarrow$ generator for $p_m(T)$ $\quad\{\mathcal{O}(mn \log n)\}$
- $(G_q, B_q) \leftarrow$ generator for $q_m(T)$ $\quad\{\mathcal{O}(mn \log n)\}$
- Compute $E \leftarrow UV^{-1}$.
- **for** $k = 1$ **to** ρ **do**
  - $E \leftarrow E \cdot E$.
- **end for**

Remark:

- Special case of construction for rational functions of Toeplitz matrices.

Scaling & Squaring for Toeplitz matrices

Input: Toeplitz matrix $T \in \mathbb{C}^{n \times n}$.
Output: Accurate approximation $E \approx \exp(T)$.

Compute $\|T\|_1$ $\{\mathcal{O}(n)\}$
Choose scaling parameter ρ and Padé approximant $r_m(z) = \frac{p_m(z)}{q_m(z)}$
Scale $T \leftarrow 2^{-\rho} T$. $\{\mathcal{O}(n)\}$
$(G_p, B_p) \leftarrow$ generator for $p_m(T)$ $\{\mathcal{O}(mn \log n)\}$
$(G_q, B_q) \leftarrow$ generator for $q_m(T)$ $\{\mathcal{O}(mn \log n)\}$
$(G, B) \leftarrow$ generator for $r_m(T) = q_m(T)^{-1} p_m(T)$ $\{\mathcal{O}(m^2 n^2)\}$
for $k = 1$ **to** ρ **do**
    $E \leftarrow E \cdot E$.
end for

Remark:

- Computation of (G, B) from G_p, B_p, G_q, B_q requires solution of $\mathcal{O}(m)$ Toeplitz-like systems of size $n \times n$.
- Fast algorithms (GKO) $\rightsquigarrow$ complexity $\mathcal{O}(m^2 n^2)$.
- Superfast alg. [Xia/Xi/Gu'2012] $\rightsquigarrow$ complexity $\mathcal{O}(m^2 n \log n)$.

Scaling & Squaring for Toeplitz matrices

Input: Toeplitz matrix $T \in \mathbb{C}^{n \times n}$.

Output: Generator (G, B) for accurate approx. $E \approx \exp(T)$.

Compute $\|T\|_1$ $\{\mathcal{O}(n)\}$

Choose scaling parameter ρ and Padé approximant $r_m(z) = \frac{p_m(z)}{q_m(z)}$

Scale $T \leftarrow 2^{-\rho} T$. $\{\mathcal{O}(n)\}$

$(G_p, B_p) \leftarrow$ generator for $p_m(T)$ $\{\mathcal{O}(mn \log n)\}$

$(G_q, B_q) \leftarrow$ generator for $q_m(T)$ $\{\mathcal{O}(mn \log n)\}$

$(G, B) \leftarrow$ generator for $r_m(T) = q_m(T)^{-1} p_m(T)$ $\{\mathcal{O}(m^2 n^2)\}$

for $k = 1$ **to** ρ **do**

    $(\tilde{G}, \tilde{B}) \leftarrow$ generator for $\mathcal{T}(G, B)^2$ $\{\mathcal{O}(m^2 n \log n)\}$

    $(G, B) \leftarrow$ compress $(\tilde{G}, \tilde{B})$ $\{\mathcal{O}(m^2 n)\}$

end for

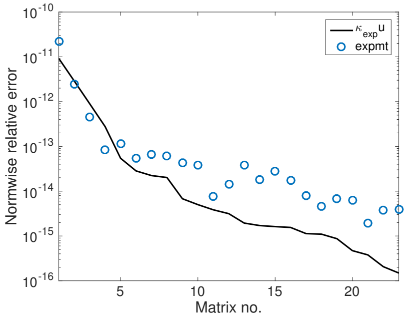
Remark:

- Recompression $=$ low-rank truncation of generator needed to avoid excessive rank growth for large ρ

Numerical experiments

Accuracy

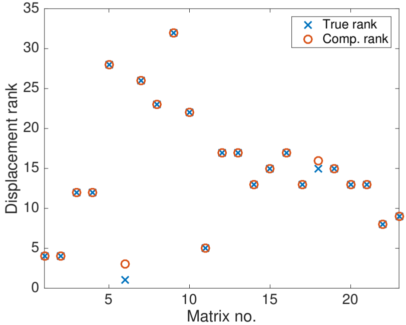
- Toeplitz matrices from the structured matrix toolbox [Redivo-Zaglia/Rodriguez'2012].
- Implementation of GKO from drsolve package [Aricò/Rodriguez'2010].



Relative error $\|\texttt{expm}(T) - \texttt{expmt}(T)\|_2 / \|\texttt{expm}(T)\|_2$.

Numerical displacement ranks

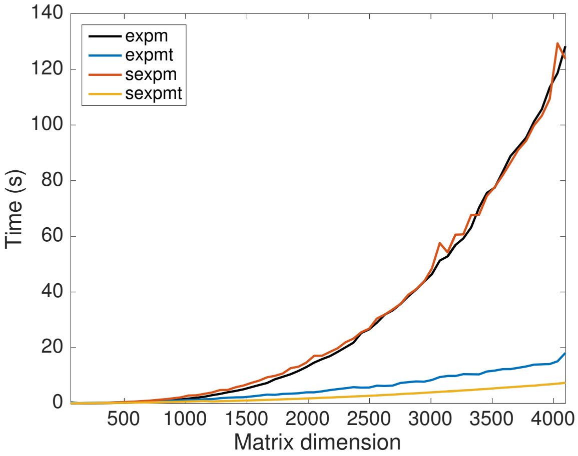
- Toeplitz matrices from the structured matrix toolbox [Redivo-Zaglia/Rodriguez'2012].
- Implementation of GKO from drsolve package [Aricò/Rodriguez'2010].



Numerical displacement ranks of `expm`(T) and `expmt`(T).

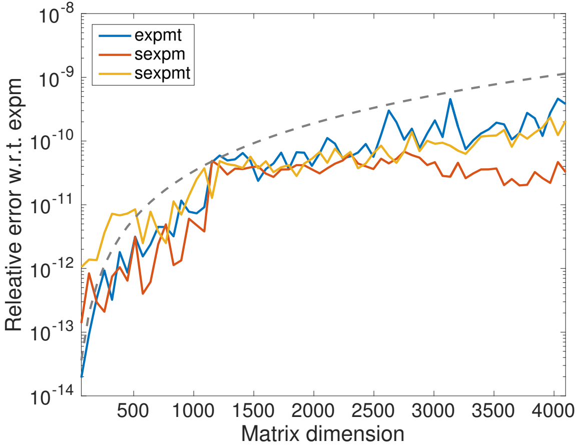
Execution time for Merton model

- Parameters of Merton model chosen as in [Lee/Pang/Sun'2010].



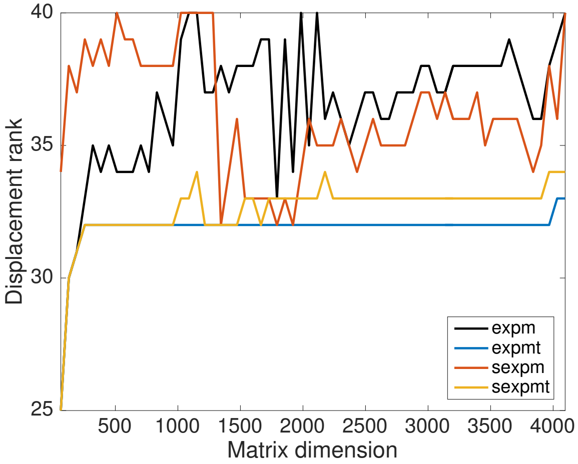
Accuracy for Merton model

- Parameters of Merton model chosen as in [Lee/Pang/Sun'2010].



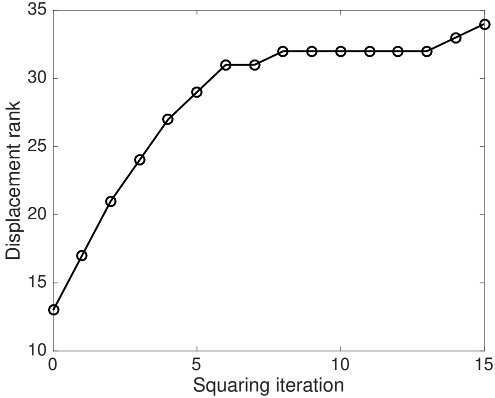
Numerical displacement rank for Merton model

- Parameters of Merton model chosen as in [Lee/Pang/Sun'2010].



Numerical displacement rank for Merton model

- Parameters of Merton model chosen as in [Lee/Pang/Sun'2010].



Evolution of displacement ranks during squaring phase for $n = 4\,096$.

Conclusions

- $\mathcal{O}(n^2)$ algorithm for exp(Toeplitz) based on approximate displacement rank and careful adaptation of scaling & squaring.
- Could be reduced to $\mathcal{O}(n \log n)$.
- Various extensions possible (other matrix functions, other structures).

More details in

- DK and Robert Luce. Fast computation of the matrix exponential for a Toeplitz matrix, 2016. Available from `http://anchp.epfl.ch`.