Time-stepping of low-rank approximations with small singular values

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Outline

Abstract

We consider low-rank approximation of time-dependent problems.

When singular values in the solution tend to zero, standard time-stepping schemes for low-rank approximation of differential equations break down.

We prove that, under mild assumptions, a new time-stepping scheme is robust in this situation.

What we are after

We want to solve parabolic and Schrödinger-type PDEs in high dimensions,

$$(-\mathrm{i})u_t = \Delta u + f(x,u), \quad x \in \mathbb{R}^d.$$

This has been done with low-rank methods,

- MCTDH[1] (Tucker format) standard approach for TDSE.
- Multi-level MCTDH[2] ($\sim$ Hierarchical Tucker) for higher dimensions.
- Tensor trains have also been used.

It seems to work, also for "real" problems, but theory is incomplete.

[1] Meyer et al. (1990)
[2] Wang and Thoss (2003)

What we are after

For most of this talk, we will stick to the ODE

$$\dot{A}(t) = F(t, A(t)), \qquad A(0) = A_0, \quad A(t) \in \mathbb{C}^{n \times n}.$$

The low-rank manifold

The set

$$\mathcal{M}_r = \{X \in \mathbb{C}^{n\times n} : \mathrm{rank}(X) = r\}$$

is a smooth manifold, embedded in $\mathbb{C}^{n\times n}$.
However, its curvature depends in a nasty way on σ_r:

$X, Y \in \mathcal{M}_r$, $\sigma_r(X) \geq \rho > 0$, $\|X - Y\| \leq \frac{1}{8}\rho$,
$B \in \mathbb{C}^{n\times n}$,
$P(X)$ orthogonal projection onto $T_X\mathcal{M}_r$. Then,[3]

$$\|(P(Y) - P(X))B\| \leq 8\rho^{-1}\|Y - X\|\|B\|_2.$$

[3] Koch and Lubich (2007).

Conflict of interests

- If σ_r small, approximation manifold strongly curved.
- If σ_{r+1} large, approximation error large.
- Reasonably, $\sigma_r \approx \sigma_{r+1}$.

Dynamical low-rank approximation

Consider the matrix ODE

$$\dot{A}(t) = F(t, A(t)), \qquad A : [0, T] \to \mathbb{C}^{n \times n}.$$

We seek a low-rank approximation $Y(t) \in \mathcal{M}_r$ to $A(t)$.
Y represented as skinny SVD,

$$Y = USV^*, \qquad U, V \in \mathbb{C}^{n \times r}, \qquad S \in \mathbb{C}^{r \times r}.$$

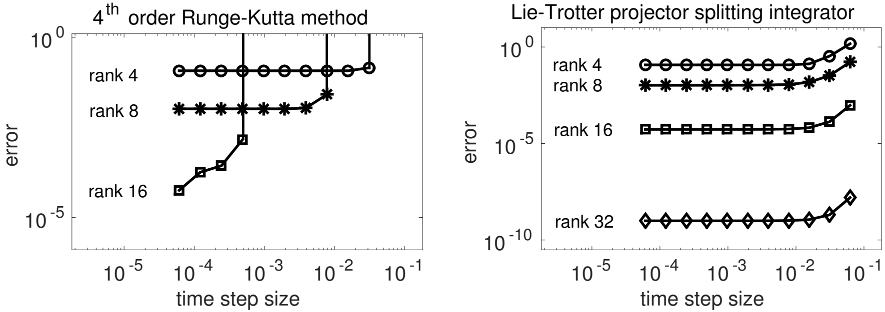
Gauge conditions $U^* \dot{U} = V^* \dot{V} = 0$ yields

$$\begin{aligned} \dot{U} &= (I - UU^*)F(t, Y)VS^{-1}, \\ \dot{S} &= U^* F(t, Y)V, \\ \dot{V} &= (I - VV^*)F(t, Y)^* US^{-*}. \end{aligned}$$

– Breaks down when $\sigma_r(Y) \to 0$. *Not a feasible way.*

Illustration of the stiffness

$$\dot{A} = W_1 A + A + A W_2^T, \qquad A(0) = \mathrm{diag}\,\{2^{-j}\}, \qquad W_i + W_i^T = 0.$$



Low-rank evolution equation

We have

$$\dot{A}(t) = F(t, A(t)), \qquad A(0) = A_0, \qquad A(t) \in \mathbb{C}^{n \times n},$$

which we approximate by

$$Y(t) \in \mathcal{M}_r = \{Y \in \mathbb{C}^{n \times n} \ : \ \mathrm{rank}(Y) = r\}.$$

Apply the Dirac–Frenkel time-dependent variational principle, i.e., a Galerkin condition on the tangent space.

Let $P(Y)$ orthogonal projection onto $T_Y\mathcal{M}_r$, and

$$\dot{Y}(t) = P(Y(t))F(t, Y(t)), \qquad Y(0) = Y_0.$$

Equivalently, find $\dot{Y}(t) \in T_Y\mathcal{M}_r$ such that

$$\langle Z, \dot{Y}(t)\rangle = \langle Z, F(t, Y(t))\rangle \quad \forall Z \in T_{Y(t)}\mathcal{M}_r.$$

Low-rank evolution equation

$$\dot{Y}(t) = P(Y(t))F(t, Y(t)), \qquad Y(0) = Y_0.$$

Compact storage of the form $Y = USV^*$.

Lipschitz constant of $P(Y)$ is proportional to the curvature of $\mathcal{M}_r$, and thus to σ_r^{-1}.

Standard time-stepping schemes break down as $\sigma_r \to 0$.

The splitting scheme

$P(Y)$ has the representation[4]

$$P(Y) = P_1^+(Y) - P_1^-(Y) + P_2^+(Y), \qquad \text{with}$$

$$P_1^+(Y)Z = ZVV^*, \quad P_1^-(Y)Z = UU^*ZVV^*, \quad P_2^+(Y)Z = UU^*Z.$$

Let $F_i^{\pm}(t, Y) = \pm P_i^{\pm}(Y)F(t, Y)$.

Then, the splitting scheme[5] reads

$$Y_1 = \Phi_{F_2^+}(h, 0, \Phi_{F_1^-}(h, 0, \Phi_{F_1^+}(h, 0, Y_0))).$$

[4] Koch and Lubich (2007).
[5] Lubich and Oseledets (2014).

The splitting scheme

More practically stated,

- $\dot{K}(t) = F(t, K(t)V_0^*)V_0, \qquad K(0) = U_0 S_0,$
- $[U_1, \widehat{S}_1] = \mathrm{qr}(K(h)),$
- $\dot{S}(t) = -U_1^* F(t, U_1 S(t) V_0^*) V_0, \qquad S(0) = \widehat{S}_1,$
- $\tilde{S}_0 = S(h),$
- $\dot{L}(t) = F(t, UL(t)^*)^* U_1, \qquad L(0) = V_0 \tilde{S}_0^*,$
- $[V_1, S_1^*] = \mathrm{qr}(L(h)).$

– Singular vectors preserved during some substeps.

For an accurate low-rank solution

- Must exist $X(t) \in \mathcal{M}_r$ such that $\|A(t) - X(t)\|$ is small (approximability).
- Approximation $Y(t)$ must be close to $X(t)$ (or $A(t)$).
- Time-stepping must be accurate, $Y_k \approx Y(kh)$ with h the time step.

We assume approximability and prove the rest, i.e.,
we show that $\|A(kh) - Y_k\|$ is small.

What we assume

$F(t, Y)$ maps almost onto the tangent space,

$$F(t, Y) = M(t, Y) + R(t, Y),$$

where

$$M(t, Y) \in T_Y \mathcal{M}_r \quad \text{and} \quad \|R(t, Y)\| \leq \varepsilon \quad \text{for all } Y \in \mathcal{M}_r.$$

For the initial data, we assume $\|Y_0 - A_0\| \leq \delta$.

We also assume that $F(t, \cdot\,)$ is Lipschitz continuous and bounded,

$$\|F(t, Y) - F(t, \tilde{Y})\| \leq L\|Y - \tilde{Y}\| \quad \text{for all } Y, \tilde{Y} \in \mathbb{C}^{n \times n},$$
$$\|F(t, Y)\| \leq B \quad \text{for all } Y \in \mathbb{C}^{n \times n}.$$

The exactness result

Theorem (Lubich and Oseledets (2014))

If

$$\dot{A}(t) = F(t), \qquad A(0) = A_0,$$

with $A(t) \in \mathcal{M}_r$ *for all* $t \in [0, T]$, *and if* $Y(0) = A_0$, *then the splitting scheme is exact.*

A similar exactness result holds also for tensor trains.

Proof (Lubich and Oseledets (2014))

We have

$$
\begin{aligned}
A_1 &= A_0 + \Delta A, \qquad A_0, A_1 \in \mathcal{M}_r, \\
Y_0 &= A_0 = U_0 S_0 V_0^*, \\
U_1 U_1^* A_1 = A_1&, \qquad A_0 V_0 V_0^* = A_0.
\end{aligned}
$$

Then, one step of the splitting scheme gives

$$
\begin{aligned}
Y_1 &= U_1 S_1 V_1^* \\
&= U_0 S_0 V_0^* + \Delta A V_0 V_0^* - U_1 U_1^* \Delta A V_0 V_0^* + U_1 U_1^* \Delta A \\
&= A_0 + (A_1 - A_0) V_0 V_0^* - U_1 U_1^* (A_1 - A_0) V_0 V_0^* + U_1 U_1^* (A_1 - A_0) \\
&= A_0 + A_1 V_0 V_0^* - A_0 - A_1 V_0 V_0^* + U_1 U_1^* A_0 + A_1 - U_1 U_1^* A_0 \\
&= A_1.
\end{aligned}
$$

□

The error estimate

Theorem

Under the stated assumptions, the error of the splitting scheme at $t_k = kh$ is bounded by

$$\|Y_k - A(t_k)\| \leq c_0\delta + c_1\varepsilon + c_2 h, \qquad t_k \leq T,$$

where c_i depend only on L, B, and T.

Standard error analysis for splitting methods, in contrast, would give an error estimate of the form

$$\|Y_k - Y(t_k)\| \leq c_0\delta + c_3\frac{h}{\varepsilon}.$$

Proof idea

For the local error estimate,

1. Construct $X(t)$, with $\dot{X}(t) = M(t, X(t))$, close to $A(t)$.
2. Show that $R(t, Y)$ introduces small perturbation in each substep.
3. Use preservation of singular vectors to isolate the perturbations, get splitting scheme for $\dot{X}$ plus perturbation.
4. Apply exactness result for $\dot{X}$.

The difficult part

Let

$$X(t) = \Phi_M(t, 0, X_0) \in \mathcal{M}_r,$$

with $\|X_0 - Y_0\| \leq h(4BLh + 2\varepsilon)$, be the solution to the problem with $R = 0$.

Lemma

Under the same assumptions as previously, we have

$$\|Y_1 - X(h)\| \leq h(9BLh + 4\varepsilon).$$

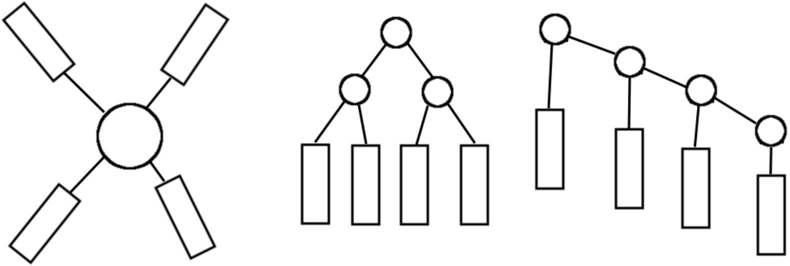
Given that...

- We assumed $\|X(0) - Y_0\| = h\,\mathcal{O}(\varepsilon + h)$.
- The lemma gives $\|Y_1 - X(h)\| = h\,\mathcal{O}(\varepsilon + h)$.
- By Grönwall's lemma, $\|\Phi_F(h, 0, Y_0) - X(h)\| \leq \mathrm{e}^{Lh}\|X(0) - Y_0\| + h\varepsilon\mathrm{e}^{Lh}$.
- $\Rightarrow$ local error $\|\Phi_F(h, 0, Y_0) - Y_1\| = h\,\mathcal{O}(h + \varepsilon)$.
- By $\|Y_0 - A_0\| \leq \delta$ and a Lady Windermere's fan argument, global error $= \mathcal{O}(\delta + h + \varepsilon)$.

In higher dimensions

Low-rank representations of the tensor
$A \in \mathbb{C}^{n_1 \times \cdots \times n_d}$:

Tucker | Hierarchical Tucker | Tensor train



$r^d + drn$ | $drn + dr^3$ | $dr^2 n$ dofs.

Extension to tensor trains

Projection to tangent space of TT-manifold reads

$$P(Y) = \sum_{i=1}^{d-1} (P_i^+(Y) - P_i^-(Y)) + P_d^+(Y), \qquad \text{with}$$

$$P_i^+ = P_{\leq i-1} P_{\geq i+1}, \quad P_i^- = P_{\leq i} P_{\geq i+1}.$$

Corresponding splitting scheme has $2d - 1$ substeps.

Elements of a tensor can be arranged in a matrix (matrix unfolding).

TT splitting scheme can be written as sequence of matrix splitting schemes.

Extension to tensor trains

Write the d-dimensional tensor Y as the matrix $Y^{\langle 1 \rangle}$, with first mode as rows and other $(d-1)$ modes as columns.

Action of d-dimensional TT splitting scheme:

- Apply first two steps of matrix splitting scheme.
- Solve third step approximately using $(d-1)$-dimensional TT splitting scheme.
- $\Rightarrow$ Error estimate follows by induction.

This can be done without forming the matrices explicitly.

Numerical example

Quantum harmonic oscillator in 2d,

$$\mathrm{i}u_t(x,t) = -\frac{1}{2}\Delta u(x,t) + V(x)u(x,t), \qquad x \in \mathbb{R}^2,\ t > 0,$$
$$u(x,0) = \pi^{-1/2}\exp\left(\frac{1}{2}x_1^2 + \frac{1}{2}(x_2-1)^2\right),$$

$$\text{with} \quad V(x) = \frac{1}{2}x^T\begin{pmatrix} 2 & -1 \\ -1 & 3 \end{pmatrix}x.$$

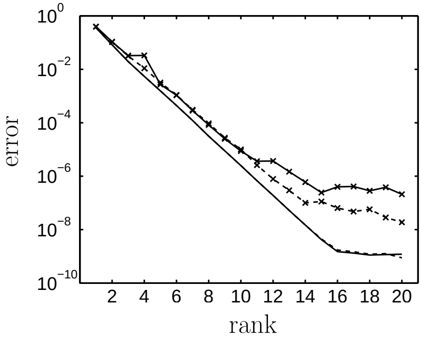
Discretise with Fourier collocation, solve subproblems with Krylov subspace method.

Lipschitz constant is nasty, $\sim \Delta x^{-2}$.

Numerical example

Since the error estimate involve the Lipschitz constant, we should need tiny time steps for PDEs ($h \ll \Delta x^2$).

Experimental experience suggests otherwise.



$n = 64$ (dashed), $n = 128$ (solid).
$h = 0.02$ ($\times$), $h = 0.01$ (plain).

Summary and outlook

- Low-rank manifolds are strongly curved where singular values are small. This makes time-integration difficult.
- For the projector-splitting integrator we proved an $\mathcal{O}(h+\varepsilon)$ error estimate, independent of the included singular values.
- Such an estimate is not possible for standard methods, as $\mathrm{Lip}(P(\cdot)) \sim \sigma_r^{-1}$.
- Estimate depends on $L = \mathrm{Lip}(F)$, and thus not applicable for PDEs.
  - Still we get good results also for PDEs.

Proof of the lemma (1/5)

We can write

$$\begin{aligned}\dot{Y}(t) &= P(Y(t))F(t, Y(t)) \\ &= \dot{X}(t) + \Delta(t, Y(t)),\end{aligned}$$

with

$$\begin{aligned}\Delta(t, Y) = F(t, Y) - F(t, X(t)) + \\ - P^{\perp}(Y)R(t, Y) + R(t, X(t)),\end{aligned}$$

and

$$\|\Delta(t, Y(t))\| \leq L \underbrace{\|Y(t) - X(t)\|}_{\leq cBh} + 2\varepsilon \leq cBLh + 2\varepsilon.$$

– Use exactness result for $\dot{X}$ and bound effect of small perturbation Δ.

Proof of the lemma (2/5)

$$\begin{aligned}\dot{Y}_i^{\pm}(t) &= \pm P_i^{\pm}(Y_i^{\pm}(t))\Big(\dot{X}(t) + \Delta(t, Y_i^{\pm}(t))\Big) \\ &= G_i^{\pm}(t, Y_i^{\pm}(t)) \qquad + \Delta_i^{\pm}(t, Y_i^{\pm}(t)).\end{aligned}$$

By the exactness result,

$$X(h) = \Phi_{G_2^+}(h, 0, \Phi_{G_1^-}(h, 0, \Phi_{G_1^+}(h, 0, X_0))).$$

Gröbner–Alekseev lemma yields

$$Y_i^{\pm}(h) = \Phi_{G_i^{\pm}}(h, 0, Y_i^{\pm}(0)) + \underbrace{\int_0^h \partial\Phi_{G_i^{\pm}}(h, t, Y_i^{\pm}(t))\Delta_i^{\pm}(t, Y_i^{\pm}(t))\,\mathrm{d}t}_{hE_i^{\pm}},$$

$$\Rightarrow Y_1 = \Phi_{G_2^+}(h, 0, \Phi_{G_1^-}(h, 0, \Phi_{G_1^+}(h, 0, Y_0) + hE_1^+) + hE_1^-) + hE_2^+.$$

Proof of the lemma (3/5)

Let $Y = Y_i^{\pm}(t)$, $Z = \pm\Delta(t, Y_i^{\pm}(t))$, and bound the integrand

$$K_i^{\pm}(\tau) = \partial\Phi_{G_i^{\pm}}(h, \tau, Y)P_i^{\pm}(Y)Z$$
$$= \lim_{\theta\to 0} \frac{1}{\theta}\Big(\Phi_{G_i^{\pm}}(h, \tau, Y + \theta P_i^{\pm}(Y)Z) - \Phi_{G_i^{\pm}}(h, \tau, Y)\Big).$$

Using $K_i^{\pm}(h) = P_i^{\pm}(Y)Z$ and $\dot{K}_i^{\pm}(\tau) = 0$ (next slide), we get

$$\|K_i^{\pm}(t)\| = \|P_i^{\pm}(Y)Z\| = \|P_i^{\pm}(Y_i^{\pm}(t))\Delta(t, Y_i^{\pm}(t))\| \le \|\Delta(t, Y_i^{\pm}(t))\|,$$

and thereby,

$$\|E_i^{\pm}\| \le cBLh + 2\varepsilon.$$

Proof of the lemma (4/5)

Important properties of the projections:

$$P_i^{\pm}(\Phi_{F_i^{\pm}}(t,s,Y)) = P_i^{\pm}(Y) \quad \text{for all } Y \in \mathcal{M}_r,$$
$$P_i^{\pm}(Y + P_i^{\pm}(Y)Z) = P_i^{\pm}(Y) \quad \text{for all } Y \in \mathcal{M}_r, Z \in \mathbb{C}^{n\times n}.$$

Using this, the derivative of $K_i^{\pm}$ follows as

$$\begin{aligned}\dot{K}_i^{\pm}(\tau) &= -\lim_{\theta\to 0}\frac{1}{\theta}\Big(G_i^{\pm}(\tau,\Phi_{G_i^{\pm}}(h,\tau,Y+\theta P_i^{\pm}(Y)Z)) \\ &\qquad - G_i^{\pm}(\tau,\Phi_{G_i^{\pm}}(h,\tau,Y))\Big) \\ &= \mp\lim_{\theta\to 0}\frac{1}{\theta}\Big(P_i^{\pm}(\Phi_{G_i^{\pm}}(h,\tau,Y+\theta P_i^{\pm}(Y)Z))\dot{X}(\tau) \\ &\qquad - P_i^{\pm}(\Phi_{G_i^{\pm}}(h,\tau,Y))\dot{X}(\tau)\Big) \\ &= \mp\lim_{\theta\to 0}\frac{1}{\theta}\Big(P_i^{\pm}(Y)\dot{X}(\tau) - P_i^{\pm}(Y)\dot{X}(\tau)\Big) = 0.\end{aligned}$$

Proof of the lemma (5/5)

$E_i^{\pm}$ were created under the action of projections, and P_1^+ and P_2^+ are "subprojections" of P_1^-. Hence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\Phi_{G_2^+}(t,0,\tilde{Y}+hE_1^-)-\Phi_{G_2^+}(t,0,\tilde{Y})\Big)=0; \quad E_1^- = P_2^+(\tilde{Y})E_1^-,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\Phi_{G_1^+}(t,0,Y_0+hE_1^+)-\Phi_{G_1^+}(t,0,Y_0)\Big)=0; \quad E_1^+ = P_1^+(Y_0)E_1^+,$$

and $Y_1 = \Phi_{G_2^+}(h,0,\Phi_{G_1^-}(h,0,\Phi_{G_1^+}(h,0,Y_0+hE_1^+)))+hE_1^- + hE_2^+$.

By the exactness result, with $X_0 = Y_0 + hE_1^+$,

$$\begin{aligned} Y_1 &= \Phi_{G_2^+}(h,0,\Phi_{G_1^-}(h,0,\Phi_{G_1^+}(h,0,X_0)))+hE_1^- + hE_2^+ \\ &= X(h) + h(E_1^- + E_2^+), \qquad \|E_1^- + E_2^+\| \le (9BLh + 4\varepsilon). \end{aligned}$$

□