Rank-adaptive time integration of tree tensor networks

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Problem of interest

Our interest is to use tree tensor networks (TTN's) to approximate solutions of evolutionary tensor differential equations

$$\dot{A}(t) = F(t, A(t)), \quad A(t_0) = A^0 \in \mathbb{C}^{n_1 \times \cdots \times n_d}. \tag{1}$$

Such problems typically arise in quantum physics, where the high order d of the differential equation is a main challenge. Tree tensor networks are a hierarchical data sparse format to approximate tensors of high order. Our model problem will be the tensor Schrödinger equation

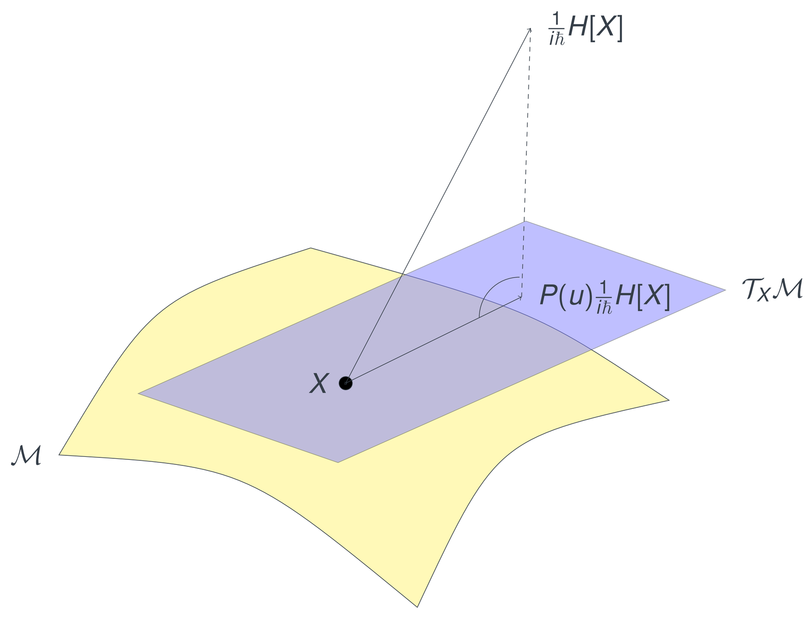
$$i\hbar \dot{A}(t) = H[A(t)]. \tag{2}$$

Dynamical low-rank approximation

On a manifold $\mathcal{M}$ we impose the time-dependent Dirac-Frenkel variational principle, see [1]: We determine $X = X(t)$ from the condition that at time t its derivative $\dot{X}$, which lies in $\mathcal{T}_X\mathcal{M}$, satisfies

$$\dot{X} \in \mathcal{T}_X\mathcal{M} \text{ such that } \langle \dot{X} - \frac{1}{i\hbar}H[X], Y\rangle = 0 \; \forall Y \in \mathcal{T}_X\mathcal{M}.$$

This can be interpreted as an orthogonal projection of the right-hand side $\frac{1}{i\hbar}H[X]$ onto the tangent space $\mathcal{T}_X\mathcal{M}$.



Tree tensor networks

Let $\mathcal{T}$ be the set of ordered trees with unequal leaves and $\mathcal{L} = \{1, \dots, d\}$ the set of leaves. Further let $\bar{\tau} \in \mathcal{T}$ be a fixed tree with d leaves. To each leaf we associate a basis matrix $\mathbf{U}_l$ and to each subtree $\tau \leq \bar{\tau}$ a connection tensor C_τ. We define a tensor $X_{\bar{\tau}}$ with a tree tensor network representation (or briefly a TTN) recursively as follows:

- ❶ For each leaf $\tau = l \in \mathcal{L}$, we set
$$X_l := \mathbf{U}_l^\top \in \mathbb{C}^{r_l \times n_l}.$$
- ❷ For each subtree $\tau = (\tau_1, \dots, \tau_m)$ (for some $m \geq 2$) of $\bar{\tau}$, we set $n_\tau = \prod_{i=1}^m n_{\tau_i}$ and $\mathbf{I}_\tau$ the identity matrix of dimension r_τ, and
$$X_\tau := C_\tau \times_0 \mathbf{I}_\tau \text{X}_{i=1}^m \mathbf{U}_{\tau_i} \in \mathbb{C}^{r_\tau \times n_{\tau_1} \times \cdots \times n_{\tau_m}},$$
$$\mathbf{U}_\tau := \mathbf{Mat}_0(X_\tau)^\top \in \mathbb{C}^{n_\tau \times r_\tau}.$$
The subscript 0 in $\times_0$ and $\mathbf{Mat}_0(X_\tau)$ refers to the mode 0 of dimension r_τ in $\mathbb{C}^{r_\tau \times r_{\tau_1} \times \cdots \times r_{\tau_m}}$.

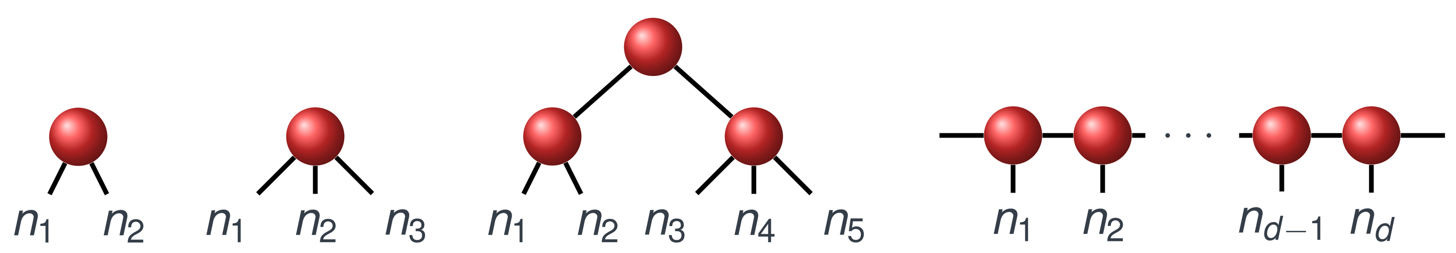


Figure: Different examples for TTN's (from left to right): matrix, Tucker tensor, general TTN, tensor train/matrix product state.

The red balls encode a connecting tensor of matching order, while the nodes n_l encode a basis matrix/leaf $\mathbf{U}_l$.

A rank-adaptive integrator for TTN's

We present a rank-adaptive integrator for tree tensor networks which extends the work of [3]. Suppose we have a TTN

$$X^0_{\bar{\tau}} = C^0_{\bar{\tau}} \times_0 \mathbf{I}_\tau \text{X}_{i=1}^m \mathbf{U}^0_{\tau_i}$$

at time t_0 and a given function F_τ, which maps a TTN to a TTN. The idea is to first update all the basis matrices $\mathbf{U}^0_{\tau_i}$ in parallel (via subflow $\Phi^{(i)}_\tau$) and then update the connecting tensor C^0_τ (via subflow Ψ_τ), i.e.

$$\widehat{X}^1_\tau = \Psi_\tau \circ (\Phi^{(1)}_\tau, \dots, \Phi^{(m)}_\tau)(X^0_\tau).$$

All the ranks of $\widehat{X}^1_\tau$ are (usually) doubled. To get the approximation X^1_τ at time t_1 we apply a truncation function θ with a given tolerance ϑ after updating the whole tree $\bar{\tau}$, i.e. $X^1_{\bar{\tau}} = \theta(\widehat{X}^1_{\bar{\tau}})$. By augmentation and truncation of the TTN at each time step the algorithm is rank-adaptive.

The subflow $\Phi^{(i)}_\tau$ applied to a TTN solves a small matrix ODE if the i-th subtree is a leaf. If the i-th subtree is again a TTN then we apply the algorithm recursively to this smaller tree.

begin
- $Y^0_{\tau_i} = X^0_{\tau_i} \times_0 S^{0,\top}_{\tau_i}$, with $\mathbf{Mat}_i(C^0_\tau)^\top = Q^0_{\tau_i} S^{0,\top}_{\tau_i}$
- **if** *$\tau_i = l$ is a leaf* **then**
  - solve $\dot{Y}_l = F_l(t, Y_l(t))$, $Y_l(t_0) = Y^0_l$
  - set $\widehat{\mathbf{U}}_l$ as an ONB of the range of $(Y_l(t_1)^\top, \mathbf{U}^0_l) \in \mathbb{C}^{n_l \times \hat{r}}$, $\hat{r}_l \leq 2r^0_l$
  - set $\widehat{M}_l = \widehat{\mathbf{U}}^*_l \mathbf{U}^0_l$
- **else**
  - $[\widehat{Y}^1_{\tau_i}, \widehat{C}^0_{\tau_i}] =$ rank-adapt-TTN-integrator $(\tau_i, Y^0_{\tau_i}, F_{\tau_i}, t_0, t_1)$
  - set $\widehat{Q}_{\tau_i}$ as an ONB of the range of $(\mathbf{Mat}_0(\widehat{C}^1_{\tau_i})^\top, \mathbf{Mat}_0(\widehat{C}^0_{\tau_i})^\top)$
  - set $\widehat{\mathbf{U}}_{\tau_i} = \mathbf{Mat}_0(\widehat{X}^1_{\tau_i})^\top$, where $\widehat{X}^1_{\tau_i}$ is obtained from $\widehat{Y}^1_{\tau_i}$ by replacing the connecting tensor with $\widehat{C}_{\tau_i} = Ten_0(\widehat{Q}^\top_{\tau_i})$
  - set $\widehat{M}_{\tau_i} = \widehat{\mathbf{U}}^*_{\tau_i} \mathbf{U}^0_{\tau_i}$

The subflow Ψ_τ solves a small tensor ODE, which can be interpreted as a Galerkin method on the updated subspace.

begin
- set $\widehat{C}^0_\tau = C^0_\tau \text{X}_{i=1}^m \widehat{M}_{\tau_i}$
- solve the tensor ODE
$$\dot{\widehat{C}}_\tau(t) = F_\tau(t, \widehat{C}_\tau(t) \text{X}_{i=1}^m \widehat{\mathbf{U}}_{\tau_i}) \text{X}_{i=1}^m \widehat{\mathbf{U}}^*_{\tau_i}, \quad \widehat{C}_\tau(t_0) = \widehat{C}^0_\tau$$
- set $\widehat{C}^1_\tau = \widehat{C}_\tau(t_1)$

Robust convergence and preserving properties

❶ Let $A(t)$ be the exact and $X^n_{\bar{\tau}}$ the numerical solution at time $t_0 + nh$. Further let $F_{\bar{\tau}}$ be Lipschitz continuous and bounded. Suppose that $||(\mathbf{I} - P(Y))F_{\bar{\tau}}(t, Y)|| \leq \epsilon \; \forall Y \in \mathcal{M}$ in a neighborhood of $A(t_n)$, where $P(Y)$ denotes the projection onto $\mathcal{T}_Y\mathcal{M}$. Then it holds
$$||A(t_n) - X^n_{\bar{\tau}}|| = \mathcal{O}(h + \epsilon + \vartheta).$$

❷ Let $A(t)$ be a continuous and differentiable family of TTN's of full tree rank $(r_\tau)_{\tau \leq \bar{\tau}}$ for $t_0 \leq t \leq t_1$. Further assume that at time t_1 all restricted subtrees $A_\tau(t_1)$ have full tree rank $(r_\sigma)_{\sigma \leq \tau}$ for all $\tau \leq \bar{\tau}$. Then for $F(t, Y) = \dot{A}(t)$ with $A(t_0) = X^0_{\bar{\tau}}$ the rank-adaptive TTN integrator is exact, i.e.
$$A(t_1) = \widehat{X}^1_{\bar{\tau}}.$$

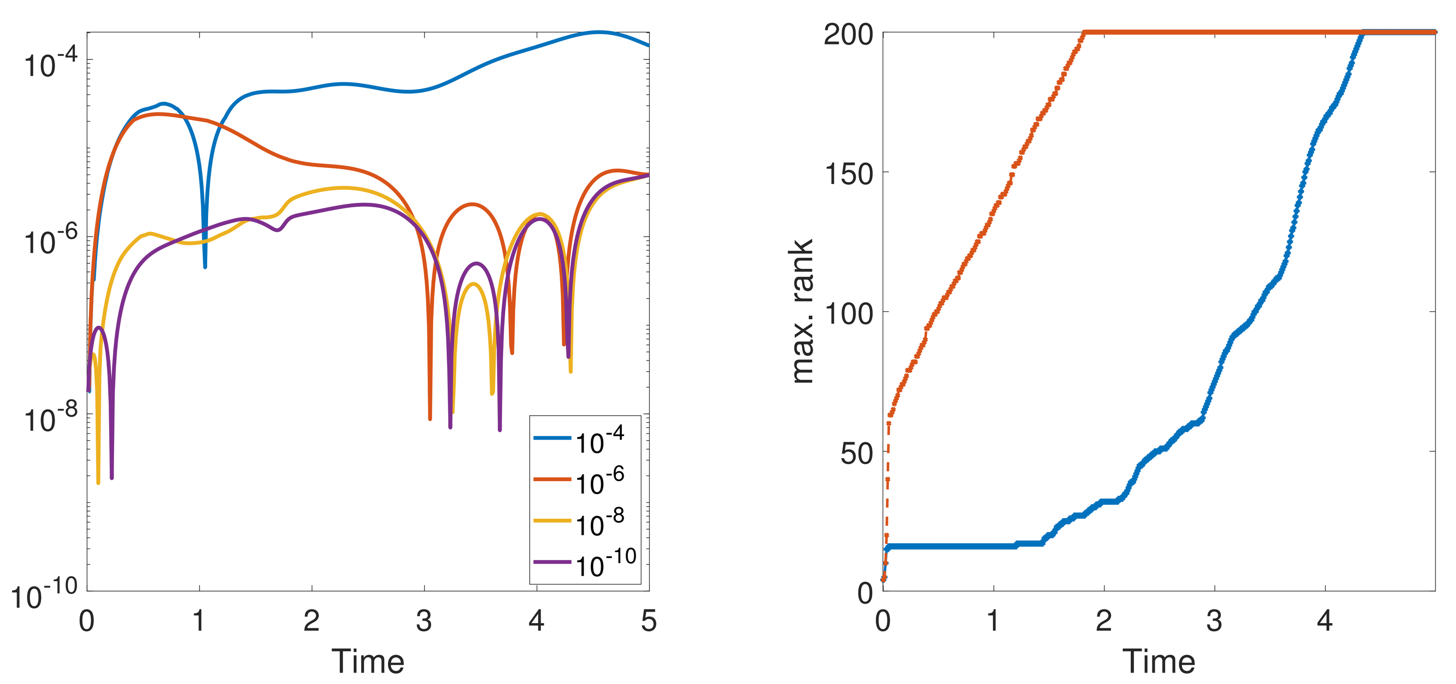
❸ If F_τ satisfies $Re\langle Y, F_{\bar{\tau}}(t, Y)\rangle = 0 \; \forall Y$ and all t, then with $c_\tau = ||C_{\bar{\tau}}||(d_{\bar{\tau}} - 1) + 1$ we have
$$\left| ||X^1_{\bar{\tau}}|| - ||X^0_{\bar{\tau}}|| \right| \leq c_{\bar{\tau}}\vartheta.$$

❹ Consider the tensor Schrödinger equation (2) and let $E(Y) = \langle Y, H[Y]\rangle$. Then it holds for every step size h
$$|E(X^1_{\bar{\tau}}) - E(X^0_{\bar{\tau}})| \leq c_{\bar{\tau}}\vartheta ||H[X^1_{\bar{\tau}} + \widehat{X}^1_{\bar{\tau}}]||.$$

Numerical experiments

We apply the integrator to a problem from quantum physics - the Ising model in a transverse field with next neighbor interaction

$$\mathrm{i}\,\partial_t \psi = H\psi \quad \text{with} \quad H = -\sum_{k=1}^d \sigma_x^{(k)} - \sum_{k=1}^{d-1} \sigma_z^{(k)}\sigma_z^{(k+1)}.$$



Left: Error of magnetization $\langle\psi|M_z|\psi\rangle = \frac{1}{d}\sum_{k=1}^d \langle\psi|\sigma_z^{(k)}|\psi\rangle$ for $\tau = 0.01$, $d = 10$ particles and different ϑ. Right: $d = 16$, $\tau = 0.01$ and $\vartheta = 10^{-8}$. Blue line gives the max. rank of a binary tree while the red line is the max. rank of a tensor train/matrix product state.

References

[1] O. Koch, Ch. Lubich. *Dynamical tensor approximation*, SIAM J. Matrix Anal. 31 (2010), 2360-2375.

[2] G. Ceruti, Ch. Lubich, D. Sulz. *Rank-adaptive time integration of tree tensor networks*, (submitted) 2022.

[3] G. Ceruti, J. Kusch, Ch. Lubich. *A rank-adaptive robust integrator for dynamical low-rank approximation*, to appear in BIT.