Numerical Linear and Multilinear Algebra in Quantum Control and Quantum Tensor Networks

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Abstract

Quantum control and quantum simulation play a key role in several applications, including quantum information processing, nanotechnology, and spectroscopy. The computational treatment of quantum problems typically involves basic tasks of numerical linear algebra. However, calculating relevant quantities of large quantum systems is a computationally demanding task as the dimension of the underlying Hilbert space—and thus also the resource requirements—grow exponentially with the size of the quantum system, in contrast to a classical configuration space just growing linearly. Therefore, classical numerical matrix approaches, which act on the entire Hilbert space, soon reach a limit, even on high-capacity hardware architectures. In order to be able to deal with larger systems and to exploit the power of today's supercomputers, numerical approaches to simulate large quantum systems require both efficient algorithms based on problem-adapted data structures and powerful hardware of (massively) parallel processors.

We address selected topics in quantum information theory from a computational perspective and exploit inherent properties of these problems in the corresponding multilinear formulation in order to develop tailored approaches and algorithms, leading to faster convergence and higher accuracy.

Numerics in a Quantum Control Algorithm

Problem Setting

- Find optimal control parameters $\boldsymbol{u}(t)$ to steer quantum-dynamical system.
- Application: Synthesization of a unitary target operator $\boldsymbol{U}_G$ with objective

$$f(\boldsymbol{U}(T),\boldsymbol{u}) \;=\; \|\boldsymbol{U}(T)-\boldsymbol{U}_G\|_F^2 \;.$$

- The dynamics are governed by the equation of motion:

$$\dot{\boldsymbol{U}}(t) \;=\; -\mathrm{i}\boldsymbol{H}(t)\boldsymbol{U}(t) \;=\; -\mathrm{i}\big[\boldsymbol{H}_0+\textstyle\sum_{m=1}^{M} u_m(t)\boldsymbol{H}_m\big]\boldsymbol{U}(t)\;.$$

GRAPE Algorithm (Khaneja, Glaser, et al., 2005)

Require: Drift Hamiltonian $\boldsymbol{H}_0$, control Hamiltonians $\boldsymbol{H}_m$, time slice $\Delta t = T/K$.
Ensure: Unitary initial state $\boldsymbol{U}_0$, unitary target gate $\boldsymbol{U}_{K+1} = \boldsymbol{U}_G^{\mathrm{H}}$.

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set initial control amplitudes u_m^{0}(t_k) for all times t_k
for ℓ = 0, 1, 2, ... until convergence do
    calculate the exponentials U_k = e^{-iΔt H(t_k)}
    compute the forward propagation U(t_k) = U_k U_{k-1} ··· U_1 U_0
    compute the backward propagation W(t_k) = U_{K+1} U_K ··· U_{k+1}
    calculate the gradient ∂f/∂u_m(t_k) = Re[trace(W(t_k)(-iΔt H_m)U(t_k))]
    update the controls u_m^{ℓ+1}(t_k) = u_m^{ℓ}(t_k) + ε · ∂f/∂u_m(t_k)
end for
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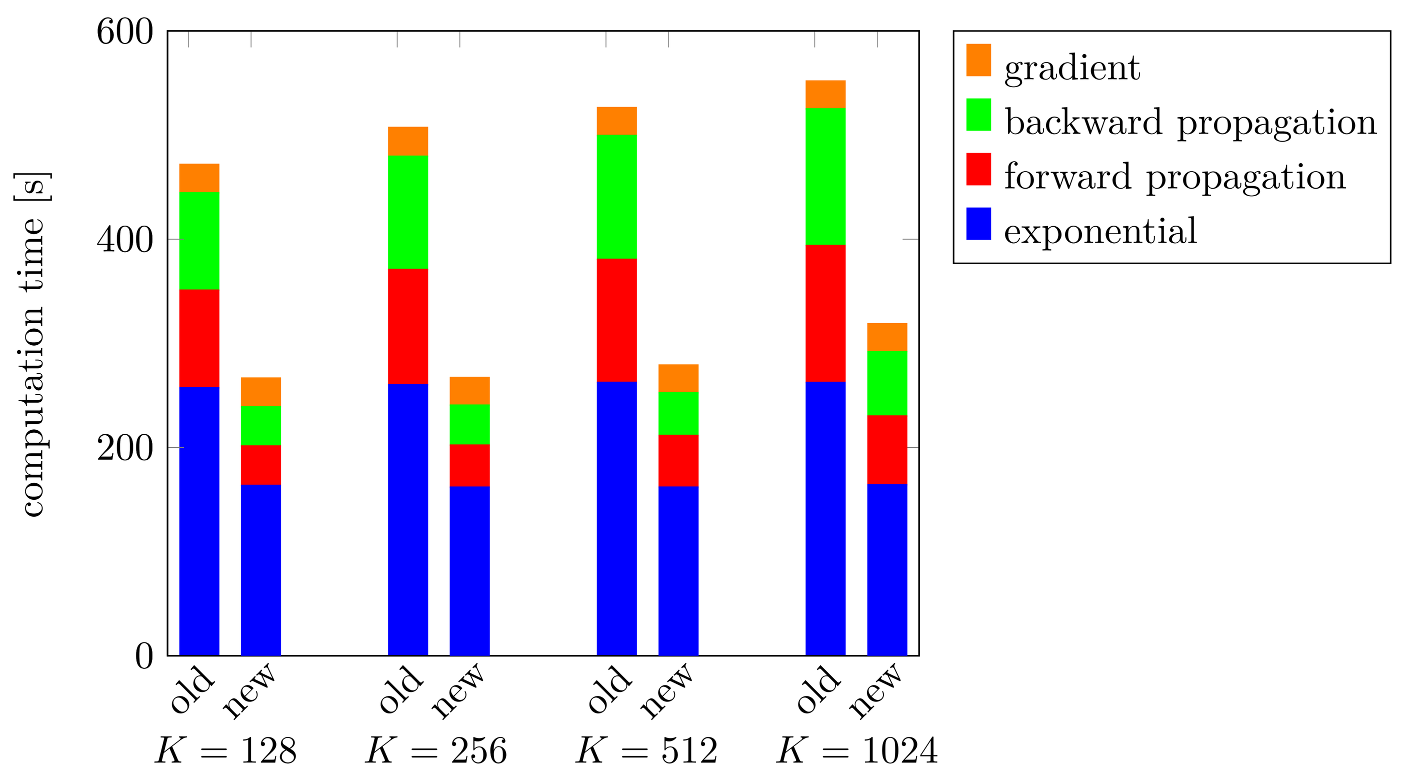
Numerical Linear Algebra Tasks

- **Matrix exponentials**
  Old: Eigendecomposition method:
  - requires dense linear algebra for typically sparse problems,
  - suffers from poor accuracy.
  New: Polynomial approach based on a Chebyshev expansion:
  + exploits sparsity of operand matrices,
  + faster convergence and higher accuracy.
- **Sequence of matrix products** (to be executed in parallel)
  Old: Prefix tree:
  - restricts the number of parallel processors,
  - increases the computational effort by a logarithmic factor.
  New: 3D Block algorithm:
  + higher flexibility in the number of processors,
  + less communication overhead.

Numerical Results (Control of 11 spin-$\frac{1}{2}$s)



Tensor Networks for Ground-State Computations

Problem Setting

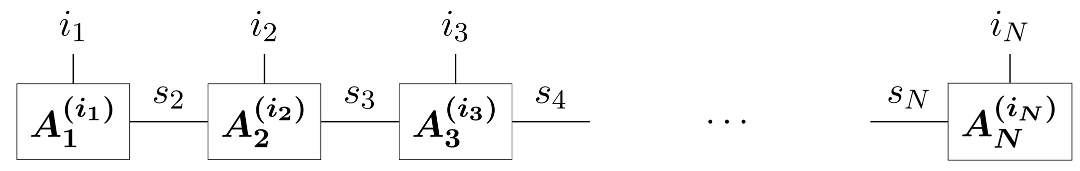
- Compute the smallest eigenvalue of the Hamiltonian $\boldsymbol{H} \in \mathbb{C}^{2^N \times 2^N}$.
- For large N neither matrices nor even vectors can be stored.
- The problem is not generic but provides certain (symmetry) properties.

Numerical Approaches

- Reformulate the eigenvalue problem as an optimization problem.
- Data-sparse representation formats reflecting the underlying coupling topology.
- Exploit symmetry relations by problem-adapted data structures and algorithms.

Approximate Representations based on Tensor Formats

- Canonical polyadic format: Cheap but unstable and without proper rank estimates.
- Tucker format: SVD-based orthogonal cores, but still exponentially expensive.
- Tensor trains (=matrix product states): Efficient **and** stable computations.



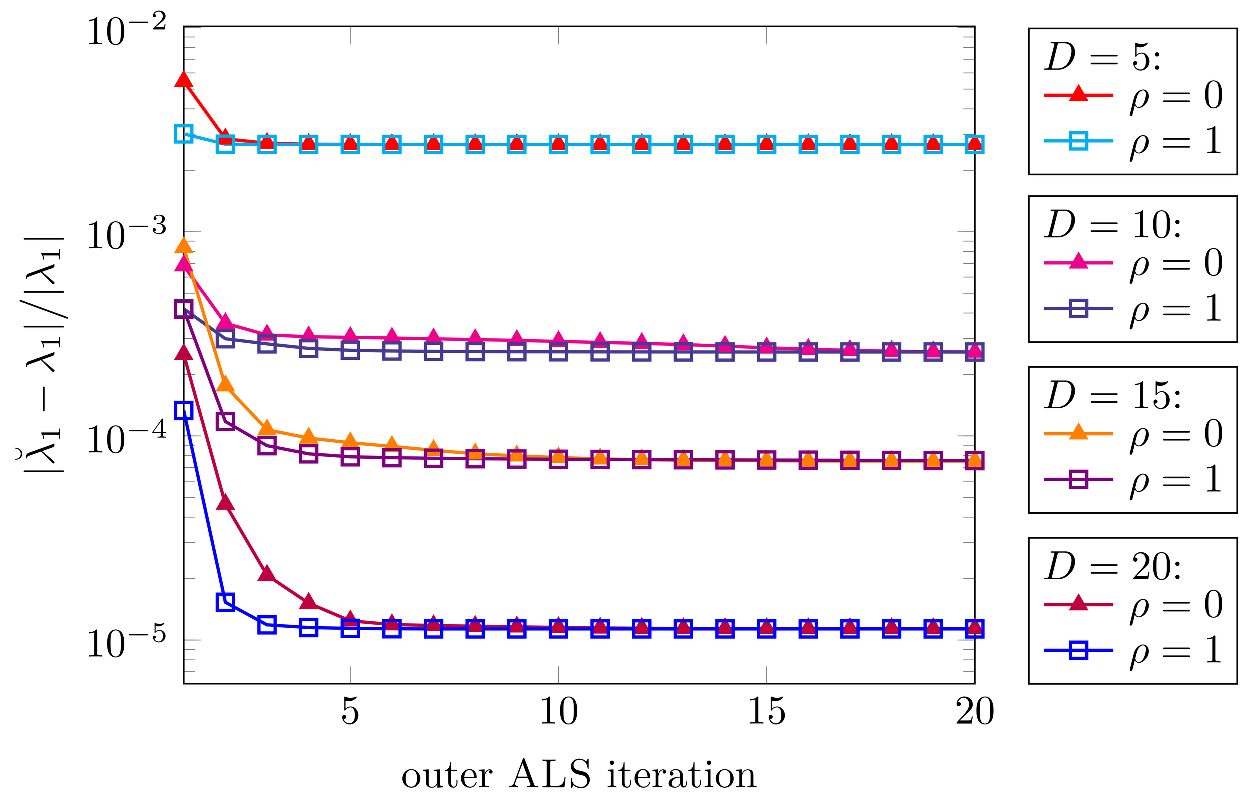
Symmetry-Adapted Representations

- Symmetric persymmetric Hamiltonian has symmetric eigenvectors $\boldsymbol{x} = \boldsymbol{J}\boldsymbol{x}$.
- Theoretical result: Vector symmetry is related to a TT representation with cores that are connected via (quasi-) involutions.
- Numerical approach: Apply established method to slightly modified Hamiltonian

$$\boldsymbol{H}(\rho) := \boldsymbol{H} + \rho(\boldsymbol{I}-\boldsymbol{J})\;.$$

$\Longrightarrow$ Faster convergence, especially in the case of degenerate eigenvalues.

Numerical Results (Ground State of the Heisenberg model)



Outlook and Further Studies

- Use low-rank tensor approaches (such as TT) to tackle quantum control problems.
- Investigate more complex quantum tensor networks.
- Develop and analyze hierarchical and hybrid tensor approaches.

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