On Riemannian quantum circuit optimization for fermionic Hamiltonian simulation

Isabel Nha Minh Le[1] and Christian B. Mendl[1,2]
[1] Technical University of Munich , School of Computation, Information and Technology [2] Technical University of Munich, Institute for Advanced Study

Classically optimize a quantum circuit to approximate the time evolution operator of a fermionic system for time Δt

- Treat the problem classically for short Δt; execute on quantum hardware for $\Delta t \gg 1$
- Use **Riemannian optimization** to incorporate the unitary constraint of the quantum gates
- Start with **fermionic swap network** that implements a Trotter step
- Approximate the reference as a higher-order Trotterization and express it as a **matrix product operator (MPO)**
- Evaluate cost function and gradient using **tensor network methods**

Quantum circuit layout and initialization

We consider fermionic Hamiltonians of the form

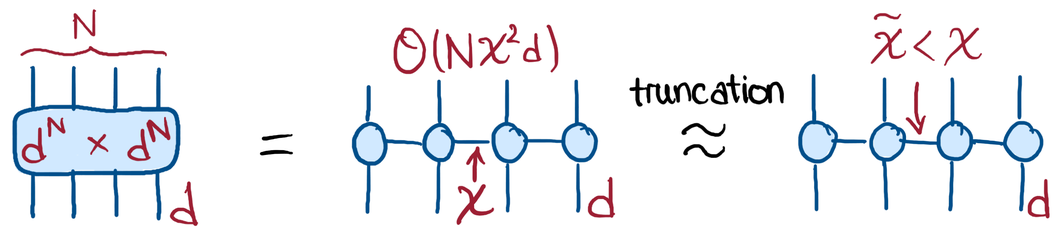
$$H = \sum_{pq} T_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pq} V_{pq} n_p n_q,$$

which covers systems like Fermi-Hubbard models or molecular Hamiltonians with diagonal interaction terms.

We initialize the model as a **fermionic swap network** [2], which implements a Trotter step using a simple brickwall circuit. E**ach orbital is represented by a qubit**. By using fermionic SWAPs, all interacting orbitals are brought next to each other once and their time evolution is given by two-qubit gates parametrized by V_{pq} and T_{pq}. We call the quantum gates $\{V_i\}$ and the quantum circuit W. Furthermore, we allow for additional layers following the brickwall circuit design.

MPO representation of the reference

To avoid the exponential scaling of the exact time evolution operator U in system size, it is useful to **factorize it into smaller tensors** and express it, e.g., as an **MPO** [3]:



An optional **truncation of the bond dimension χ** results in a lower-rank approximation of the original MPO. In practice, we compute the reference U_{MPO} as a high-accuracy approximation using 4^{th}-order Trotterization and a suitable truncation ($\varepsilon = 1e-14$).

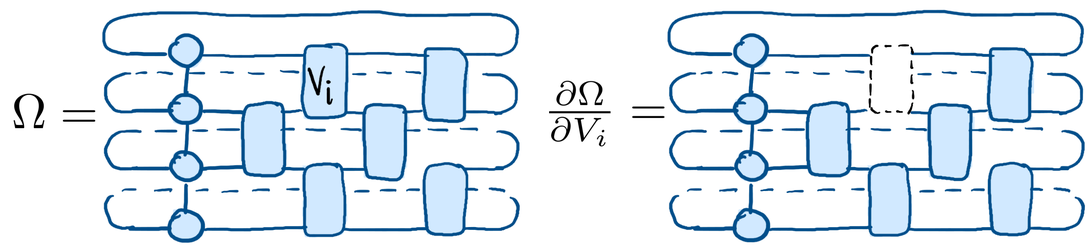
Cost function and gradient evaluation

The deviation of the quantum circuit W from the reference U_{MPO} can be quantified by the normalized Frobenius norm

$$\mathcal{L} = 2^{-N} \|U_{\mathrm{MPO}} - W\|_F^2 = 1 + 2^{-N} \left(C - 2\Re(\Omega)\right),$$

where C is the norm of the reference and $\Omega = \mathrm{Tr}(U_{\mathrm{MPO}}^\dagger W)$ is the variational part of the cost function.

By viewing the quantum circuit as a tensor network, **the cost function is evaluated by tensor network contraction**, and similarly, **the partial derivative is obtained by "cutting out" the quantum gate**:



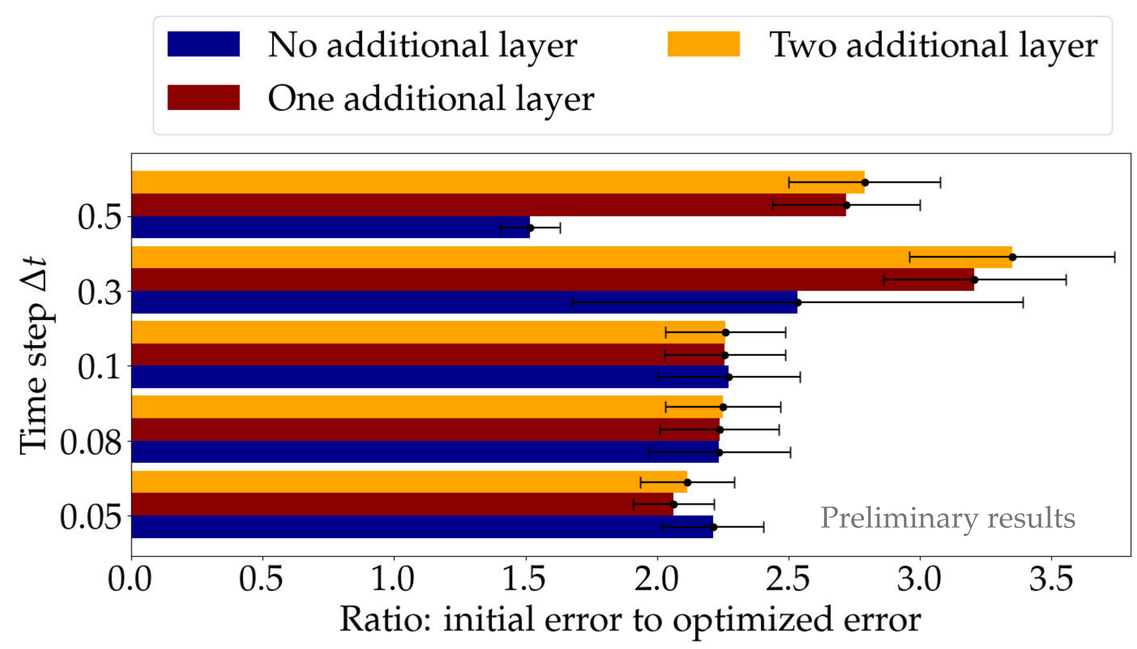
Following the above, the Euclidean gradient is computed.

Riemannian optimization of unitary quantum gates [4]

The objective is to optimize the quantum gates under **unitary constraints** using **Riemannian optimization**. The set of two-qubit gates forms a Riemannian manifold $\mathcal{U}$ with a tangent space $\mathcal{T}_V\mathcal{U}$ and an inner product $\langle X, Y\rangle_V = \mathrm{Tr}(X^\dagger Y)$ associated to each point $V \in \mathcal{U}$. The Riemannian gradient corresponds to the projection of the Euclidean gradient onto the corresponding tangent space. Within Riemannian optimization, an update step is taken into the negative direction of the Riemannian gradient. The resulting point needs to be retracted from the tangent space into the manifold by, e.g., taking the unitary part of its polar decomposition.

Numerical results (preliminary)

The following shows the relative improvement from the initial 2^{nd} order Trotterization after the optimization when using the same circuit layout (blue) and when allowing for an additional layer of two-qubit gates (red) for the Fermi-Hubbard model in 1D with 60 spin orbitals.



[1] I. N. M. Le and C. B. Mendl. "Leveraging tensor network methods and Riemannian quantum circuit optimization for fermionic Hamiltonian simulation." In prep.
[2] I. D. Kivlichan, et al. "Quantum simulation of electronic structure with linear depth and connectivity." Phys. Rev. Letters 120.11 (2018): 110501.
[3] L. Causer, et al. "Scalable simulation of nonequilibrium quantum dynamics via classically optimized unitary circuits." Phys. Rev. Research 6.3 (2024): 033062.
[4] A. Kotil, et al. "Riemannian quantum circuit optimization for Hamiltonian simulation." J. Phys. A 57.13 (2024): 135303.