Trotter error bounds and dynamic multi-product formulas for Hamiltonian simulation

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Multi-product formulas (MPF) are linear combinations of Trotter circuits offering high-quality simulation of Hamiltonian time evolution with fewer Trotter steps. Here we report two contributions aimed at making multi-product formulas more viable for near-term quantum simulations. First, we extend the theory of Trotter error with commutator scaling developed by Childs, Su, Tran et al. to multi-product formulas. Our result implies that multi-product formulas can achieve a quadratic reduction of Trotter error in 1-norm (nuclear norm) on arbitrary time intervals compared with the regular product formulas without increasing the required circuit depth or qubit connectivity. The number of circuit repetitions grows only by a constant factor. Second, we introduce dynamic multi-product formulas with time-dependent coefficients chosen to minimize a certain efficiently computable proxy for the Trotter error. We use a minimax estimation method to make dynamic multi-product formulas robust to uncertainty from algorithmic errors, sampling and hardware noise. We call this method Minimax MPF and we provide a rigorous bound on its error.

References

[1] Zhuk,S., Robertson, N, Bravyi, S. arXiv:2306, (2023)

Figures

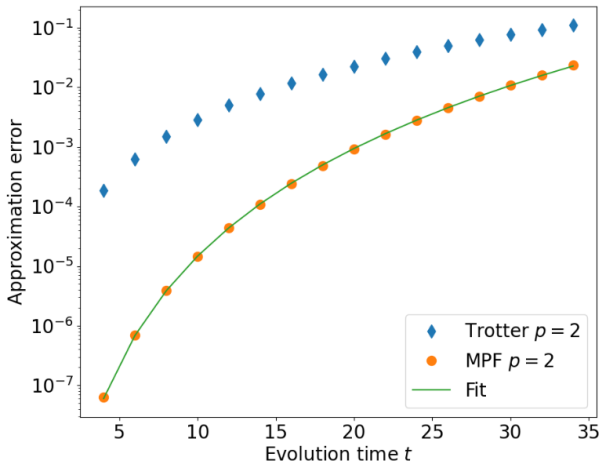

Figure 1: Approximation error achieved by the second-order Trotter circuit with k3 = 850 time steps (blue) and MPF with (k1, k2, k3) = (200, 650, 850) (orange) for the Heisenberg spin chain Hamiltonian with n = 14 qubits. Green line shows the fitting formula.

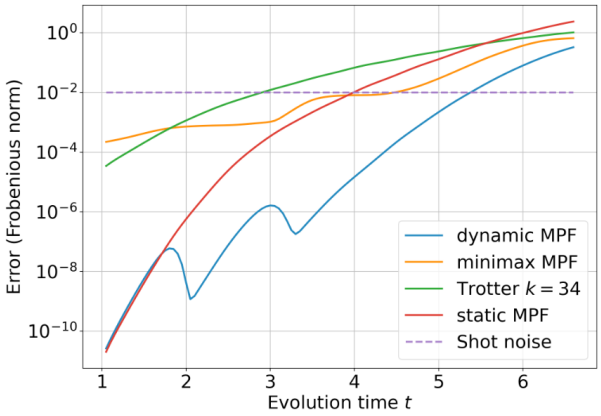

Figure 2: Approximation error for MPFs: well-conditioned static MPF with ρ8,26,34 (red), best Trotter formula ρ34(green), dynamic MPF with exact data (blue) and mini-max MPF with noisy/approximated data (orange) both using ρ8,20,26,30,34, for the Heisenberg spin chain Hamiltonian Eq. (30) with n = 10 qubits. The shot noise magnitude is depicted as a dashed line for reference.