

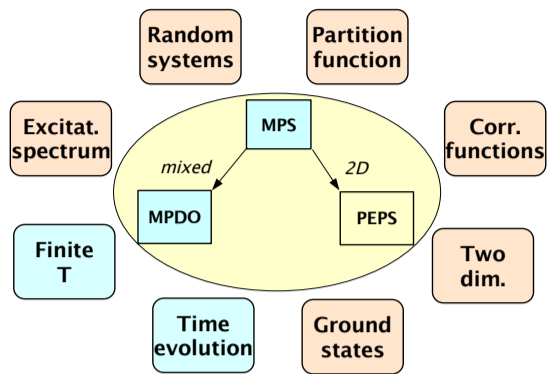


Time evolution algorithms for MPS and DMRG.

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Overview



► **Matrix Product States (MPS)** are a family of variational wavefunctions with multiple applications in the study of **low-dimensional quantum many-body systems**.

► We have developed new algorithms for simulating real and imaginary time evolution of MPS.

► We have compared these algorithms with other from MPS and DMRG.

MPS

► **Matrix Product States (MPS)** are a family of states densely distributed over the Hilbert space

$$\mathcal{S}_D := \left\{ \left(\text{Tr} \prod_k A_k^{s_k} \right) |s_1 \dots s_N\rangle, A_k^{s_n} \in \mathbb{C}^{D \times D} \right\}$$

► MPS are described by N matrices of dD^2 complex numbers, where d is the physical dimension of a site and size D is related to the accuracy.

► MPS do not form a vector space:

$$\begin{aligned} |1\rangle^{\otimes N}, |0\rangle^{\otimes N} &\in \mathcal{S}_1, \\ |0\rangle^{\otimes N} + |1\rangle^{\otimes N} &\in \mathcal{S}_2. \end{aligned}$$

It is therefore possible using linear combinations of MPS to increase the accuracy of a MPS approximation.

► MPS can be used to efficiently compute scalar products, $\langle \psi | \phi \rangle$, distances, $\| \psi - \phi \|$, and expected values $\langle \psi | O_1 \otimes O_2 \otimes \dots \otimes O_L | \phi \rangle$.

Optimal projection

► Given an arbitrary vector, the nonlinear operator \mathcal{P}_D finds the MPS of size D which best approximates it [1,2].

► It can be used to simplify a linear combination of MPS

$$\mathcal{P}_D \sum_k c_k |\phi^{(k)}\rangle := \underset{\psi \in \mathcal{S}_D}{\text{argmin}} \left\| |\psi\rangle - \sum_k c_k |\phi^{(k)}\rangle \right\|^2$$

► Also to compute the action of an operator defined as $U := X^{-1}Y$,

$$\mathcal{P}_D (X^{-1}Y|\phi\rangle) := \underset{\psi \in \mathcal{S}_D}{\text{argmin}} \|X|\psi\rangle - Y|\phi\rangle\|,$$

where X and Y are sums of products of local operators

$$X, Y := \sum_{\alpha} O_1^{\alpha} \otimes \dots \otimes O_L^{\alpha}.$$

► The optimal projection can be computed efficiently, by a sequential optimization of the state.

Trotter methods

► We work with **nearest-neighbor interactions** and decompose the Hamiltonian into odd- and even-bond terms [3]

$$H = \sum_{k=1}^{L/2} H_{2k} + \sum_{k=1}^{L/2} H_{2k-1} =: H_E + H_O.$$

► The evolution operator is then decomposed using a **Suzuki-Trotter formula**

$$U_2 := e^{-iH_E \Delta t} e^{-iH_O \Delta t} + O(\Delta t^2)$$

or a Forest-Ruth, ($1/\theta := 2 - 2^{1/3}$).

$$U_4 \simeq e^{-iH_E \theta \Delta t / 2} e^{-iH_O \theta \Delta t} e^{-iH_E (1-\theta) \Delta t / 2} \times e^{-iH_O (1-2\theta) \Delta t} e^{-iH_E (1-\theta) \Delta t / 2} e^{-iH_O \theta \Delta t} e^{-iH_E \theta \Delta t / 2},$$

► The operators are applied to the MPS. Afterwards we truncate to keep the size of matrices fixed [2,1]

$$|\psi(t + \Delta t)\rangle := \mathcal{P}_D e^{-iH_E \Delta t} e^{-iH_O \Delta t} |\psi(t)\rangle.$$

Taylor/Padé methods

► We look for higher order approximations which are not restricted to NN interactions.

► The first method is a fourth order Taylor expansion, equivalent to a Runge-Kutta method [4]

$$\begin{aligned} |\psi(\Delta t)\rangle &= \sum_{n=0}^4 \frac{1}{n!} (iH\Delta t)^n |\psi(0)\rangle + O(\Delta t^5) \\ &\simeq \prod \mathcal{P}_D (iH\Delta t - z_k) |\psi(0)\rangle, \end{aligned}$$

where $\{z_k\}$ are roots of the 4th order polynomial.

► The other methods are Padé expansions of the exponentials, including the Crank-Nicholson method and a fourth order method

$$|\psi(\Delta t)\rangle \simeq \mathcal{P}_D \frac{1 - i\Delta t H / 2 - (\Delta t H)^2 / 12}{1 + i\Delta t H / 2 - (\Delta t H)^2 / 12} |\psi(0)\rangle$$

► Both methods require of the optimal projection operator with X being the denominator and Y the numerator.

Arnoldi method

► We expand the next time step in a basis of MPS constructed out of an approximate orthogonalization of Krylov vectors

$$|\phi_{k+1}\rangle \simeq \mathcal{P}_D \left(H|\phi_k\rangle - \sum_{j \leq k} \frac{\langle \phi_j | H | \phi_k \rangle}{\langle \phi_j | \phi_j \rangle} |\phi_j\rangle \right),$$

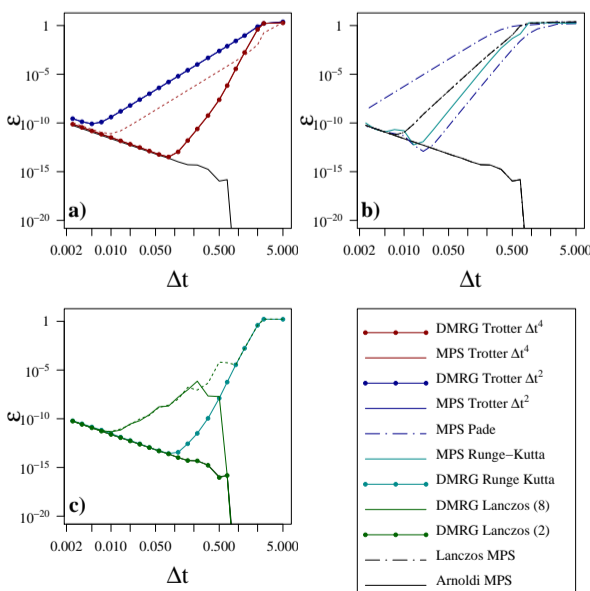
► With these vectors we estimate the Hamiltonian $N_{ik} := \langle \phi_j | \phi_i \rangle$ and $H_{ik} := \langle \phi_j | H | \phi_i \rangle$ and then write

$$|\psi(\Delta t)\rangle := \mathcal{P}_D \sum_k [e^{-i\Delta t N^{-1}H}]_{k0} |\phi_k\rangle.$$

► The main idea behind is that a **linear combination of MPS is more accurate** than a single MPS of the same size.

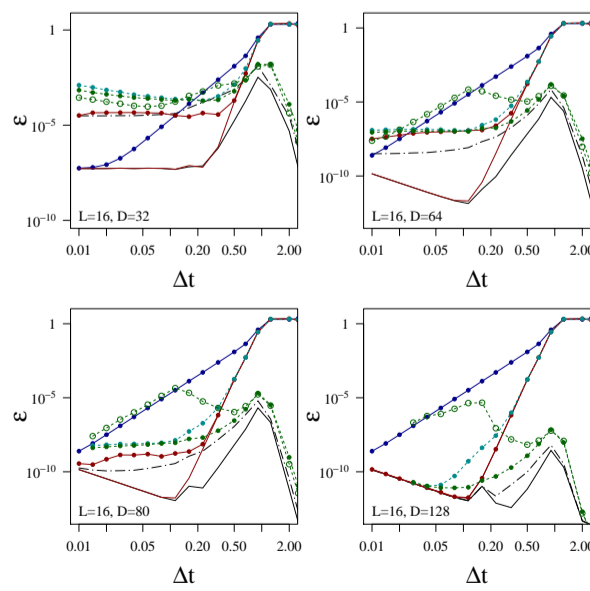
► The Arnoldi basis cannot be replaced by a Lanczos basis [5] because MPS lose orthogonality very quickly when there are truncation errors.

Without truncation



► For 8 spins and $D = 16$, there are no truncation errors and methods follow expected laws $O(\Delta t^2), O(\Delta t^4), \dots$. But if too short time step, we have important rounding errors.

Bigger problems



► For bigger systems, there are truncation errors. In that case MPS methods perform better than DMRG methods, which only converge when basis is very large.

Conclusions

► Several new numerical method for studying the evolution of Matrix Product states.

► Very accurate for long time steps, thus suitable for studying "adiabatic" processes.

► Accuracy of MPS methods proven better than DMRG equivalents.

► Huge potential for improvement: parallelizability, better ansatz, ...

Related bibliography:

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