Tensor Networks - Homework 3

Lecturer: Juan José Mendoza Arenas

All the following questions require the implementation of an ITensor algorithm. Please provide the solutions in a Jupyter Notebook.

1. TEBD for real-time evolution of XXZ spin model (35 points)

The following Hamiltonian corresponds to one of the basic models of magnetism: the XXZ spin-1/2 chain in a magnetic field along z direction and open boundary conditions.

$$H = J\sum_{j=1}^{N-1}(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + B\sum_{j=1}^{N}(-1)^j S_j^z. \tag{1}$$

The parameter J is the exchange interaction, Δ is the anisotropy, and B is the amplitude of the magnetic field. We have assumed a staggered magnetic field, which alternates signs. For the following exercise, consider $N = 24$ sites and $J = 1$.

a) Define an initial MPS in which the first half of the lattice has spins pointing up, and the second half has spins pointing down (3 points).

b) Implement a TEBD code for simulating the time evolution of the initial MPS under the Hamiltonian of Eq. (1), up to a final time $T = 8.0$. Select adequate values for the time step δt and truncation parameters (20 points).

c) Obtain the magnetization along z at every site of the spin chain for times $t = 0, 2, 4, 6, 8$, and for the following combinations of parameters Δ and B. Plot and save the results of each combination of Δ and B on a separate figure (2 points each figure).

i. $\Delta = 0$, $B = 0$. ii. $\Delta = 0$, $B = 2$. iii. $\Delta = 2$, $B = 0$.

d) Obtain the von Neumann entanglement entropy at every bond of the spin chain for times $t = 0, 2, 4, 6, 8$, and for the same combinations of parameters Δ and B of c). Plot and save the results of each combination of Δ and B on a separate figure (2 points each figure).

2. TDVP for ground state of spin model with next-nearest neighbor interactions (25 points)

As an alternative to DMRG, the ground state of a Hamiltonian H can be obtained through imaginary time evolution. As discussed by G. Vidal (Phys. Rev. Lett. **93**, 040502 (2004) and Phys. Rev. Lett. **98**, 070201 (2007)), the ground state $|\psi_0\rangle$ can be obtained as

$$|\psi_0\rangle = \lim_{\tau\to\infty}|\psi_\tau\rangle \qquad \text{with} \qquad |\psi_\tau\rangle = \frac{\exp(-H\tau)|\phi\rangle}{||\exp(-H\tau)|\phi\rangle||} \tag{2}$$

for some initial state $|\phi\rangle$ which has a non-zero overlap with $|\psi_0\rangle$, i.e., $\zeta = |\langle\phi|\psi_0\rangle| > 0$. In addition, if the Hamiltonian has a gap $\Delta > 0$, the overlap between the evolved state $|\psi_\tau\rangle$ and the ground state grows with imaginary time τ as

$$|\langle\psi_\tau|\psi_0\rangle| > 1 - \mathcal{O}\left(\frac{e^{-2\Delta\tau}}{\zeta^2}\right). \tag{3}$$

Equation (3) may become meaningless for a gapless Hamiltonian ($\Delta = 0$) of in the thermodynamic limit (system size $N \to \infty$). However, even in these cases, the imaginary time evolution method can correctly obtain $|\psi_0\rangle$, as indicated by successful benchmark calculations.

Consider the following spin-1/2 Hamiltonian with interactions between nearest (J_1) and next-nearest neighbors (J_2), and with a local magnetic field h along x direction:

$$H = J_1 \sum_{i=1}^{N-1} S_i^z S_{i+1}^z + J_2 \sum_{i=1}^{N-2} S_i^z S_{i+2}^z - h \sum_{i=1}^{N} S_j^x. \tag{4}$$

a) Using imaginary time evolution with TDVP, obtain the ground state $|\psi_0\rangle$ and ground state energy E_0 of the Hamiltonian for $N = 30$, $J_1 = 1$, $J_2 = 0.5$, and $h = 2$. Feel free to choose the initial state, time step, final time, and truncation parameters. You can compare with the results of Homework 2 to verify the correctness of your implementation (18 points).

b) Plot the evolution of the energy as a function of the imaginary time τ (5 points).

b) Calculate and plot the ground state expectation values $\langle S_j^x \rangle$ for all sites j (2 points).

3. TDVP for solution of Burgers' equation (25 points)

Consider the velocity $u(x, t)$ of a one-dimensional flow. Burgers' equation has the form

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{1}{\mathrm{Re}}\frac{\partial^2 u}{\partial x^2}, \tag{5}$$

with Re the Reynolds number. Consider a system with $N = 8$ qubits, spatial range $0 \leq x < 1$, $\mathrm{Re} = 1000$, time step $\Delta t = 10^{-3}$, final time $T = 0.24$ and a Gaussian initial condition given by

$$u(x, 0) = \exp(-8\pi(x - 1/2)^2). \tag{6}$$

Note that the parameters satisfy the stability condition $\Delta t \leq (\mathrm{Re}/2)\Delta x^2$.

a) Solve Burgers' equation using TDVP (22 points).

b) In a single figure, plot the results of $u(x, t)$ as a function of x for truncation parameter $\chi = 8$ and times $t = 0, 0.06, 0.12, 0.18, 0.24$. You can compare with the results of Homework 2 to verify the correctness of your implementation (3 points).

4. Fit Algorithm for solution of Burgers' equation (15 points)

a) Solve Burgers' equation, with the same initial condition and parameters as in the previous exercise, using the DMRG-like Fit algorithm (12 points).

b) In a single figure, plot the results of $u(x, t)$ as a function of x for truncation parameter $\chi = 8$ and times $t = 0, 0.06, 0.12, 0.18, 0.24$. You can compare with the results of Homework 2 and of the previous exercise to verify the correctness of your implementation (3 points).