Tensor Networks - Homework 2

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1. Function derivatives using MPO-MPS product (25 points)

For the first two questions, please provide the analytical development. For the last three questions, please use a system of $N = 8$ qubits, and provide the solution in a Jupyter Notebook.

a) Obtain the MPO for the right shift operator with periodic boundary conditions (5 points).

b) Obtain the MPO for the identity operator with periodic boundary conditions (5 points).

c) Calculate the first derivative of the function $f(x) = \cos^2(x)$ in the range $0 \leq x < 2\pi$, using an eight-order central finite difference (5 points).

d) Calculate the second derivative of the function $f(x) = \cos^2(x)$ in the range $0 \leq x < 2\pi$, using an eight-order central finite difference (5 points).

e) Calculate the overlap between the normalized MPS results of c) and d), and the normalized analytical results encoded as MPS (5 points).

2. MPS solution of Burgers' equation (25 points)

Burgers' equation is one of the simplest nonlinear equations in fluid dynamics. Consider the velocity $u(x,t)$ of a one-dimensional flow. Here, Burgers' equation has the form

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

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

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

Note that the parameters satisfy the stability condition $\Delta t \leq (\mathrm{Re}/2)\Delta x^2$. To solve Burgers' equation using MPS, follow the outlined steps. Please provide the solution in a Jupyter Notebook.

a) Encode the initial condition as an MPS, and define the derivative operators as MPOs using eight-order central finite difference (2 points).

b) Implement a time loop for calculating $u(x, t + \Delta t)$ from $u(x,t)$, approximating the time derivative as (first order forward finite difference)

$$\frac{\partial u}{\partial t} \approx \frac{u(x, t + \Delta t) - u(x,t)}{\Delta t}. \tag{3}$$

Note that the Hadamard product is necessary for the nonlinear term of the equation (15 points).

c) In a single figure, plot the results of $u(x,t)$ as a function of x for truncation parameter $\chi = 8$ and times $t = 0, 0.06, 0.12, 0.18, 0.24$ (4 points).

d) Which is the minimal truncation parameter χ for obtaining good results? (4 points).

3. MPOs of Hamiltonians of many-body systems (15 points)

a) Consider the following spin-1/2 Hamiltonian with interactions between nearest and next nearest neighbors, and with a local magnetic field:

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

Here, S_i^z and S_i^x are z and x spin operators acting on site i of a lattice of N spins. For a system of $N = 4$, show that the MPO of the Hamiltonian is given by the following tensors:

$$W^{[1]} = \begin{bmatrix} -hS^x & J_1 S^z & J_2 S^z & I \end{bmatrix}, \quad W^{[i]} = \begin{bmatrix} I & 0 & 0 & 0 \\ S^z & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ -hS^x & J_1 S^z & J_2 S^z & I \end{bmatrix}, \quad W^{[N]} = \begin{bmatrix} I \\ S^z \\ 0 \\ -hS^x \end{bmatrix}. \tag{5}$$

Here, I is a 2×2 identity matrix, and 0 is the 2×2 zero matrix. Note the intermediate identity inserted in the bulk tensor to implement the next-nearest neighbor Hamiltonian (7 points).

b) Evidence with an example that an exponentially decaying interaction $J(r) = Je^{-r/\xi} = J\lambda^r$, where $r > 0$ and $\lambda = \exp(-1/\xi)$, can be captured by an MPO with bulk tensor (8 points)

$$W^{[i]} = \begin{bmatrix} I & 0 & 0 \\ S^z & \lambda I & 0 \\ 0 & J\lambda S^z & I \end{bmatrix}. \tag{6}$$

4. DMRG of spin-1/2 Hamiltonian (35 points)

Consider the spin-1/2 Hamiltonian given Eq. (4), with $N = 30$, $J_1 = 1$, $J_2 = 0.5$, and $h = 2$.

a) Implement the MPO using the OpSum function of ITensor. Note that the required spin operators S^α ($\alpha = x, z$) can be found in $S = 1/2$ and Qubit SiteTypes (3 points).

b) Define an initial MPS which encodes the antiferromagnetic state $|\uparrow\downarrow\uparrow\downarrow \cdots \uparrow\downarrow\rangle$ (3 points).

c) Calculate the ground state $|\psi_0\rangle$ and ground state energy E_0 of the Hamiltonian, using DMRG and the antiferromagetic state as starting point. You are free to decide on the following parameters: number of sweeps, values of bond dimension χ, values of cutoff error, and tolerance of convergence of energy (15 points).

d) Check convergence to an eigenstate by evaluating the variance of the Hamiltonian (5 points).

e) Calculate and plot the ground state expectation values $\langle S_j^x \rangle$ for all sites j of the system (3 points).

f) Calculate and plot (as a heat mat) the ground state correlations $\langle S_j^z S_k^z \rangle$ for all pairs of sites j, k of the system (3 points).

g) Calculate the first excited state $|\psi_1\rangle$, first excited state energy E_1, and the energy gap $E_1 - E_0$ of the Hamiltonian (3 points).