Sheet 3: Matrix-product states

Released: 05/19/23; Submit until: 06/09/23 (**20 Points**)

Matrix-product states (MPS) are maybe the most successful framework for studying one-dimensional systems. In the following, we will set up a small toolkit that implements the an important property of MPS: The compression of wave functions. To achieve that goal, we need a few ingredients that allow us to work with rank-3 tensors, which are at the heart of representing wave functions as MPS.

Problem 1 Fusing and splitting **(4 Points)**

Consider a set of rectangular matrices $\mathbf{M}^k \in \mathbb{V}_{\mathbb{K}}^{m\times n}$ ($\mathbb{K} = \mathbb{R}, \mathbb{C}$) where $k \in \{0, \dots, d-1\}$ for some $d \in \mathbb{N}$. Writing for each k the matrices component-wise $M^k_{\alpha,\beta}$, we define a left (right) fusion by merging the index k with the index α (β):

$$\text{Left fusion: } M_{(k,\alpha),\beta} \in \mathbb{V}_{\mathbb{K}}^{d\cdot m\times n}\ , \quad \text{Right fusion: } M_{\alpha,(k,\beta)} \in \mathbb{V}_{\mathbb{K}}^{m\times d\cdot n}\ . \tag{1}$$

The fused indices are mapped to a new index via $(k, \alpha) = k \cdot m + \alpha$ and $(k, \beta) = k \cdot n + \beta$ and can be realized by stacking the matrices M^k either vertically, or horizontally. Similarly, we define the left (right) splitting by decomposing the fused indices

$$\text{Left splitting: } k = (k,\alpha) \operatorname{div} m\ , \qquad \alpha = (k,\alpha) \bmod m \tag{2}$$

$$\text{Right splitting: } k = (k,\beta) \operatorname{div} n\ , \qquad \beta = (k,\beta) \bmod n\ , \tag{3}$$

where div denotes the integer division and mod the modulo operation. For both operations of index fusing and splitting, write two functions performing the left and write fusing and splitting. For the fusion operation, the functions map a set of matrices to a bigger matrix: $M^k_{\alpha,\beta} \longmapsto M_{(k,\alpha),\beta}$. For the splitting operation, the functions map a big matrix into a set of smaller matrices: $M_{(k,\alpha),\beta} \longmapsto M^k_{\alpha,\beta}$. Write reasonable test cases to ensure the correct functionality of your implementations.

Problem 2 Matrix-product states and the canonical form **(8 Points)**

A matrix-product state is simply a collection of sets of matrices (rank-3 tensors) that is, to each lattice site we are assigning such a set $M^{k_j}_{\alpha_{j-1},\alpha_j}$. Note that the index $j \in \{0, \dots, L-1\}$ is introduced to label the different matrix dimensions α_j, α_j and matrices k_j at the different sites and L denotes the number of lattice sites. Such a matrix-product state allows to represent the coefficients of a wave function $c_{k_0,k_1,\dots,k_{L-1}} \in \mathbb{K}$ on a tensor-product Hilbert space:

$$|\psi(\{\mathbf{M}^{k_j}\})\rangle = \sum_{k_0,\dots,k_{L-1}} \underbrace{\mathbf{M}^{k_0} \cdot \mathbf{M}^{k_1} \cdots \mathbf{M}^{k_{L-1}}}_{c_{k_0,k_1,\dots,k_{L-1}}} |n_{k_0}, \dots, n_{k_{L-1}}\rangle\ , \tag{4}$$

where $|n_{k_j}\rangle$ are the basis states of the jth degress of freedom. In particular, for spin systems we have $d = 2$ with $|n_{k_j=0} =\downarrow\rangle$ and $|n_{k_j=1} =\uparrow\rangle$.

(2.a) **(3P)** Implement a class `MPS` that contains a collection of L such sets of matrices $M^{k_j}_{\alpha_{j-1},\alpha_j}$. These matrices should have dimensions $m_j \leq m$ and we will call $m \in \mathbb{N}$ the maximum bond dimension. Note that at the ends of the MPS, i.e., $j = 0$ and $j = L - 1$, the matrix dimensions have to be such that the overall MPS contracts to a number: $\alpha_0 = \alpha_L \equiv 1$. The parameter m should be a property of the MPS class. Also write a method that initializes the set of site matrices either via input parameters, or with random numbers.

(2.b) **(5P)** In order to perform numerical optimizations we use the canonical form. It is defined by fixing the additional gauge degrees of freedom of the MPS-representation via:

$$\text{Left orthogonal:} \quad \sum_{(k_j,\alpha_{j-1})} M^{\dagger}_{(k_j,\alpha_{j-1}),\alpha_j} M_{(k_j,\alpha_{j-1}),\beta'_j} = \delta_{\alpha_j,\alpha'_j} \tag{5}$$

$$\text{Right orthogonal:} \quad \sum_{(k_j,\alpha_j)} M_{\alpha_{j-1},(k_j,\alpha_j)} M^{\dagger}_{\alpha'_{j-1},(k_j,\alpha_j)} = \delta_{\alpha_{j-1},\alpha'_{j-1}} \tag{6}$$

Note that these conditions can be evaluated easily as matrix-matrix product of left-/right-fused matrices. In practice, we fix the gauge by performing a singular value decomposition (SVD) of the left-/right-fused matrices

$$\text{Left orthogonal:} \ M_{(k_j,\alpha_{j-1}),\alpha_j} = \sum_{s_j} U_{(k_j,\alpha_{j-1}),s} S_{s_j} V_{s_j,\alpha_j} \ , \tag{7}$$

$$\text{Right orthogonal:} \ M_{\alpha_{j-1},(k,\alpha_j)} = \sum_{s_j} U_{\alpha_{j-1},s_j} S_{s_j} V_{s_j,(k,\alpha_j)} \ . \tag{8}$$

For each gauge, implement a function which performs an SVD on the fused matrices of a given site. For the left orthogonal gauge, replace the set of site matrices with the set of splitted U-matrices: $M^{k_j}_{\alpha_{j-1},\alpha_j} \longleftarrow U^{k_j}_{\alpha_{j-1},s_j}$ and multiply the remainder of the SVD to the set of site matrices to the right: $M^{k_{j+1}}_{\alpha_j,\alpha_{j+1}} \longleftarrow \sum_{\alpha_j} S_{s_j} V_{s_j,\alpha_j} M^{k_{j+1}}_{\alpha_j,\alpha_{j+1}}$. Accordingly, for the right orthogonal gauge, replace the set of site matrices with the set of splitted V-matrices: $M^{k_j}_{\alpha_{j-1},\alpha_j} \longleftarrow V^{k_j}_{s_j,\alpha_j}$ and multiply the remainder of the SVD to the set of site matrices to the left: $M^{k_{j-1}}_{\alpha_{j-2},\alpha_{j-1}} \longleftarrow \sum_{\alpha_{j-1}} M^{k_{j-1}}_{\alpha_{j-2},\alpha_{j-1}} U_{\alpha_{j-1},s_j} S_{s_j}$.

Don't forget to write test cases that ensure the correct orthogonality properties of the set of site matrices.

Problem 3 Compression of wave functions **(8 Points)**

The canonical form can be used to efficiently represent quantum-many body states by maximizing the overlap between a guess state $|\tilde{\psi}\rangle$ and the target state $|\psi\rangle$. In order to simplify the notation, we denote those sets of site matrices satisfying the left-orthogonal condition by $\mathbf{A}^{k_j}$ and those satisfying the right-orthogonal condition by $\mathbf{B}^{k_j}$. We furthermore denote the left fusion of a set of site-matrices by adding an arrow to the left: $\overleftarrow{\mathbf{M}}_j$ and correspondingly denote the right fusion of a set of site matrices by adding an arrow to the right: $\overrightarrow{\mathbf{M}}_j$. Note that using that notation we have $\overleftarrow{\mathbf{A}}^{\dagger}_j = \overrightarrow{\mathbf{A}}^{*}_j$ and $\overrightarrow{\mathbf{B}}^{\dagger}_j = \overleftarrow{\mathbf{B}}^{*}_j$ where the star denotes the adjoint matrix, as well as:

$$\overrightarrow{\mathbf{A}}^{*}_j \overleftarrow{\mathbf{A}}_j = \mathbb{1}_{m_j \times m_j} \quad \text{and} \quad \overrightarrow{\mathbf{B}}_j \overleftarrow{\mathbf{B}}^{*}_j = \mathbb{1}_{m_{j-1} \times m_{j-1}} \ . \tag{9}$$

Finally, we define the mixed-canonical form of a wave function with gauge-center j via

$$|\psi(j)\rangle = \sum_{k_0,\ldots,k_{L-1}} \mathbf{A}^{k_0}\cdots\mathbf{A}^{k_{j-1}}\mathbf{M}^{k_j}\mathbf{B}^{k_{j+1}}\cdots\mathbf{B}^{k_{L-1}}\,|n_{k_0},\ldots,n_{k_{L-1}}\rangle \ . \tag{10}$$

We can therefore write the overlap between two states $|\psi\rangle\,,|\tilde{\psi}\rangle$ as

$$\langle\tilde{\psi}|\psi\rangle = \mathrm{Tr}\sum_{k_j}\left(\tilde{\mathbf{M}}^{k_j}\right)^{\dagger}\overset{\rightarrow}{\tilde{\mathbf{A}}}{}^{*}_{j-1}\cdots\overset{\rightarrow}{\tilde{\mathbf{A}}}{}^{*}_{0}\overset{\leftarrow}{\mathbf{A}}_0\cdots\overset{\leftarrow}{\mathbf{A}}_{j-1}\mathbf{M}^{k_j}\overset{\rightarrow}{\mathbf{B}}_{j+1}\cdots\overset{\rightarrow}{\mathbf{B}}_{L-1}\overset{\leftarrow}{\tilde{\mathbf{B}}}{}^{*}_{L-1}\cdots\overset{\leftarrow}{\tilde{\mathbf{B}}}{}^{*}_{j+1}\ , \tag{11}$$

where fused matrix sets with a tilde belong to the state $|\tilde{\psi}\rangle$. Optimization of the cost function $\||\psi\rangle - |\tilde{\psi}\rangle\|$ with respect to the coefficients $\tilde{M}^{k_j}_{\alpha_{j-1},\alpha_j}$ of the guess state then yields the equation

$$\overset{\rightarrow}{\tilde{\mathbf{A}}}{}^{*}_{j-1}\cdots\overset{\rightarrow}{\tilde{\mathbf{A}}}{}^{*}_{0}\overset{\leftarrow}{\mathbf{A}}_0\cdots\overset{\leftarrow}{\mathbf{A}}_{j-1}\mathbf{M}^{k_j}\overset{\rightarrow}{\mathbf{B}}_{j+1}\cdots\overset{\rightarrow}{\mathbf{B}}_{L-1}\overset{\leftarrow}{\tilde{\mathbf{B}}}{}^{*}_{L-1}\cdots\overset{\leftarrow}{\tilde{\mathbf{B}}}{}^{*}_{j+1} = \tilde{\mathbf{M}}^{k_j}\ , \tag{12}$$

which provides us with an update rule for the coefficients $\tilde{\mathbf{M}}^{k_j}$ of the guess state. Note that the updates can be made very efficient using the recursive structure of the contractions of left- and right-orthogonal fused site matrices.

(3.a) **(1P)** Write a sweep function which prepares a state in a mixed-canonical form such that the gauge center is at a given target site j.

(3.b) **(3P)** Extend your sweep function such that it works on two input states. While sweeping to the right, moving the gauge center from $j \to j+1$, calculate the contraction $\Omega_L^j = \overset{\rightarrow}{\tilde{\mathbf{A}}}{}^{*}_{j}\Omega_L^{j-1}\overset{\leftarrow}{\mathbf{A}}_j$ where Ω_L^{j-1} is the result of the previous contraction and $\Omega_L^{-1} = 1$. Implement the same operation for a left sweep moving the gauge center from $j \to j-1$: $\Omega_R^j = \overset{\rightarrow}{\mathbf{B}}_j\Omega_R^{j+1}\overset{\leftarrow}{\tilde{\mathbf{B}}}{}^{*}_{j}$ with $\Omega_R^L = 1$. You need to keep track of the sequence of transfer matrices $\left\{\Omega_L^{-1},\ldots\Omega_L^{j-1}\right\}$ and $\Omega_R^{j+1},\ldots,\Omega_R^L$

(3.c) **(4P)** You can now evaluate eq. (12) recursively, starting from two states with gauge center at site $j=0$ and update every set of site matrices $\tilde{\mathbf{M}}^{k_j} \longleftarrow \Omega_L^{j-1}\mathbf{M}^{k_j}\Omega_R^{j+1}$. At each lattice site, you can easily evaluate the overlap using the transfer matrices: $\langle\tilde{\psi}|\psi\rangle = \mathrm{Tr}\,\tilde{\mathbf{M}}^j\Omega_L^{j-1}\mathbf{M}^j\Omega_R^{j+1}$. Use your split-, fuse and SVD-functions, to convert ground states of the transverse field Ising model from the previous exercise, at intermediate couplings $h \sim \mathcal{O}(1)$ into a matrix-product state as discussed in the lecture. Vary the max. bond dimensions m of your guess state and for each value of m, plot the overlap after two subsequent sweeps (left-to-right and right-to-left). How many sweeps do you need to converge the approximation? How does the overlap (approximation quality) depend on m?