Matrix Product States

Glenn LeBlanc, Karthik Siva *

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Introduction

Many-Body Wavefunctions as Tensors

Consider a spin-$\frac{1}{2}$ particle. The particle's state is given by $|\psi\rangle \in \mathbb{C}^2$, and for some computational basis $\{|0\rangle, |1\rangle\}$ we can write

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$$

with

$$|\alpha|^2 + |\beta|^2 = 1.$$

This is the principle of superpostion– the particle is superposed between the two basis states $|0\rangle$ and $|1\rangle$. Now if we add a second spin-$\frac{1}{2}$ particle, the many-body system $|\Psi\rangle$ is in some superposition of the four states

$$|\Psi\rangle = \alpha |00\rangle + \beta |01\rangle + \gamma |10\rangle + \delta |11\rangle .$$

Generally, for N qubits (qudits) the system is fully parameterized by 2^N (d^N) complex numbers: $|\Psi\rangle \in \mathbb{C}^{2^N}$. Notice the exponential scaling here. It is useful also to notice the natural bijection between the two spaces

$$\mathbb{C}^{2^N} \longleftrightarrow \mathbb{C}^{2\times\cdots\times 2}$$

meaning we can instead conceptualize $|\Psi\rangle$ as a *tensor*:

$$|\Psi\rangle \in \mathbb{C}^{2\times\cdots\times 2}$$

where in this paper a tensor Ψ is just a multi-dimensional array with some number of indices such that plugging in an assignment for each index spits out a complex number. More succinctly,

$$\Psi_{i_1,i_2,\cdots,i_N} \in \mathbb{C}$$

A *contraction* between two tensors Ψ and Φ is a summation over a shared index:

$$T_{i,j,l,m} = \sum_k \Psi_{i,j,k}\Phi_{l,k,m}$$

is an example of a contraction. Note that dot products, matrix multiplication, and trace are all different vestiges of tensor contraction:

$$a \cdot b = \sum_k a_k b_k$$

$$(Ax)_i = \sum_k A_{ik} x_k$$

$$\mathrm{Tr}(A) = \sum_k A_{kk}$$

Tensor Networks

A *tensor network* is an undirected graph whose nodes represent tensors and whose edges correspond to tensor indices. An edge between two tensors corresponds to a contraction along the depicted axis of each tensor. Use of this graphical language for representing quantum systems is attractive since it unveils relevant entanglement properties [1].

*This project was part of the Berkeley Physics Directed Reading Program, which allows undergraduates to explore novel material under the auspices of a graduate student mentor. K. Siva very graciously directed this project.

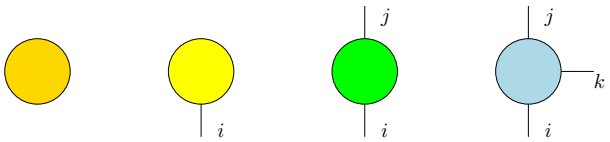

Figure 1: *A graphical depiction of a scalar c, vector v_i, matrix M_{ij}, and a tensor T_{ijk} of rank three.*

See figure 1 for a graphical depiction of tensors of rank zero to three. Each tensor is denoted as a node with free edges representing each index.

Figure 2 depicts the previous examples (dot product, matrix multiplication, trace) of tensor contraction using this graphical language.

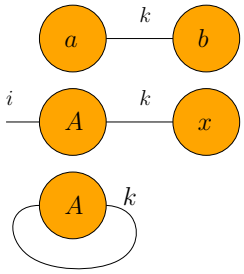

Figure 2: *A graphical depiction of three examples of tensor contraction.*

An example of an insight this graphical language provides is in proving trace cyclicality. The standard proof is as follows:

$$\begin{aligned}\mathrm{Tr}(ABC) &= \sum_{ijk} A_{ij}B_{jk}C_{ki} \\ &= \sum_{ijk} C_{ki}A_{ij}B_{jk} \\ &= \mathrm{Tr}(CAB)\end{aligned}$$

The tensor network proof is depicted in figure 3:

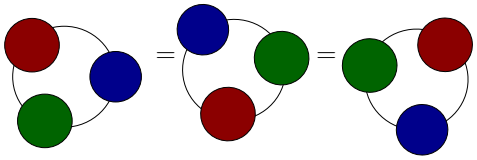

Figure 3: *Proof of trace cyclicality.*

The graphical depiction of trace provides simpler insight into the cyclic structure of the underlying tensor contractions required to calculate $\mathrm{Tr}(ABC)$, and thus allows for a totally visual and immediately obvious proof of the invariance of trace under cyclic permutations of A, B, and C.

Matrix Product States

A *matrix product state* (MPS) is a particular class of tensor network consisting of a chain of tensors each having one dangling edge and a bond between their nearest neighbors. See figure 4 for an example of a MPS with three sites with periodic and nonperiodic boundary conditions. From here we only consider MPS with nonperiodic boundary conditions.

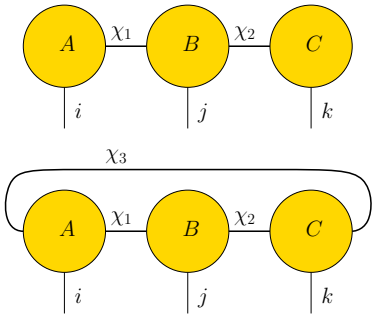

Figure 4: *Two three-site MPS, the first lacking periodic boundary conditions and the second with periodic boundary conditions.*

The indices χ_i in figure 4 are called *bond indices* and are associated with a *bond dimension*. The free indices i, j, k are *site indices*. Algebraically, the MPS decomposition of a tensor Ψ is written as:

$$\Psi_{i_1,i_2,\cdots,i_N} = \sum_{\chi_1,\chi_2,\cdots,\chi_{N-1}} A_{i_1}^{[1]\chi_1} A_{i_2}^{[2]\chi_1,\chi_2} \cdots A_{i_N}^{[N]\chi_{N-1}}$$

where the first and last local tensors $A^{[1]}$ and $A^{[N]}$ are matrices and every other tensor in the chain is of rank three. If each bond index is constrained to be of the same dimension χ then this representation approximates the 2^n coefficients of Ψ using

$$2\chi + (N-2)2\chi^2 + 2\chi = 4\chi + (2N-4)\chi^2$$

parameters, which grows as $O(N)$ for fixed χ. For a given choice of site indices (e.g., $i_1 = 0$, $i_2 = 1$, $i_3 = 0$, $\cdots$), the coefficient $\Psi_{010\cdots}$ is given by a matrix product– hence the name matrix product state.

Consider a state $|\Psi\rangle \in \mathbb{C}^{2\times\cdots\times 2}$ associated with N qubits. The *Schmidt decomposition* of $|\Psi\rangle$ with respect to a partition of sites $A : B$ is written

$$|\Psi\rangle = \sum_{\alpha}^{\chi_A} \lambda_\alpha |\Phi_\alpha^{[A]}\rangle \otimes |\Phi_\alpha^{[B]}\rangle$$

where χ_A is the *Schmidt rank* of the partition $A : B$ and is a natural measure of the entanglement between the qubits in A and those in B [2]. If $\max_A \chi_A = \chi$ and

$$2^N > 4\chi + (2N-4)\chi^2,$$

then the MPS decomposition of $|\Psi\rangle$ with uniform bond dimension χ is exact and requires less memory than storing the individual 2^N coefficients of $|\Psi\rangle$.

Generating a MPS from a tensor

The first step of the iterative process for generating a MPS from a tensor is depicted in figure 6 for an initial tensor with three indices, each of dimension d. The input tensor ψ is reshaped into a matrix ψ_{MAT} by squashing indices the two leftmost indices into one index while keeping the rightmost index separated. The singular value decomposition is then performed on ψ_{MAT}. Σ is truncated and renormalized to Σ' such that the bond index between V and Σ is less than or equal to the bond dimension χ. The truncated matrix Σ' is contracted to the left into U, resulting in the $d^2 \times \chi$ matrix ψ'_{MAT}. Finally, the index of dimension d^2 is unsquashed into two indices of dimension d each. The process is repeated for ψ', with the only change being that the middle site index is squashed with the bond index and the leftmost site index is kept separate. This process is repeated iteratively for every site index in the original tensor ψ until the tensor corresponding to the leftmost site is the only untouched tensor. See figure 5 for a depiction of this iterative process.

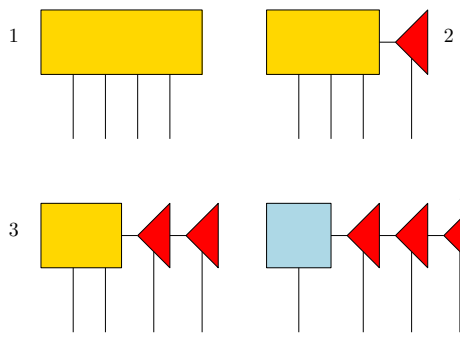

Figure 5: *How a MPS is generated using iterative SVD with an input tensor with four indices. Steps are numbered accordingly. The final orthogonality center is in blue.*

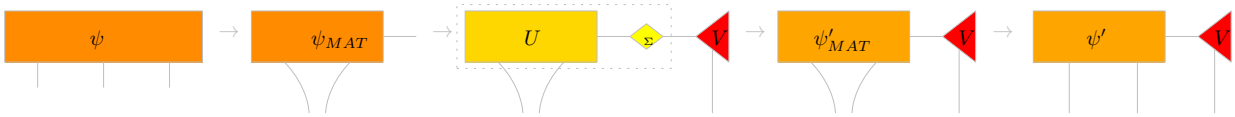

Figure 6: *Separating the first site index from ψ.*

The leftmost site in figure 6 is an orthonormal matrix by definition of the SVD. Non-boundary sites in the final chain resulting from iteratively applying this method are *right normal*, which is a loose generalization of orthonormality. Algebraically, if a tensor $T_{L,i,R} \in \mathbb{C}^{b\times d\times b}$ is right normal, then

$$\sum_{i,R} T_{L,i,R} T^*_{L',i,R} = \delta_{L,L'}$$

and likewise if T is left normal then

$$\sum_{i,L} T_{L,i,R} T^*_{L,i,R'} = \delta_{R,R'}.$$

See figure 7 for a graphical depiction of this property.

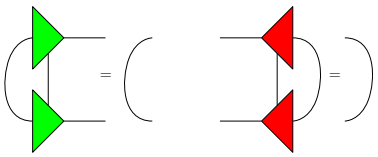

Figure 7: *Left normality (green) and right normality (red).*

If a MPS consists entirely of a nonnegative (possibly zero, as in figure 5) number of left normal tensors facing a single unconstrained tensor followed by a chain of right normal tensors we call the single unconstrained tensor the *orthogonality center.*

Moving the Orthogonality Center

The orthogonality center presents a useful way of evaluating the expectation of a local operator M on site i, depicted in figure 8.

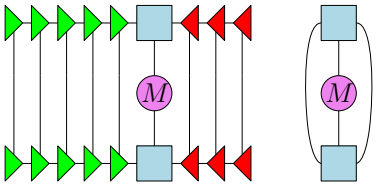

Figure 8: *A quick way to find $\langle M^{(i)} \rangle_\psi$ exploiting orthogonality. Left: the full contraction equivalent to $\langle \psi_{MPS} | M^{(i)} | \psi_{MPS} \rangle$. Left and right normal tensors can be removed, leaving the contraction on the right as the only necessary computation.*

However, this requires that the orthogonality center is already located on site i. Since this clearly will not always be the case, we need a way to move the orthogonality center from one site to another. The general idea is depicted in figure 9. Briefly, the orthogonality center's site index is squashed with the left (right) bond index. Next it is split into two matrices using the QR (LQ) decomposition, and the left (right) normal matrix is reshaped into a rank three tensor. The remaining matrix is contracted into the corresponding right (left) neighbor tensor.

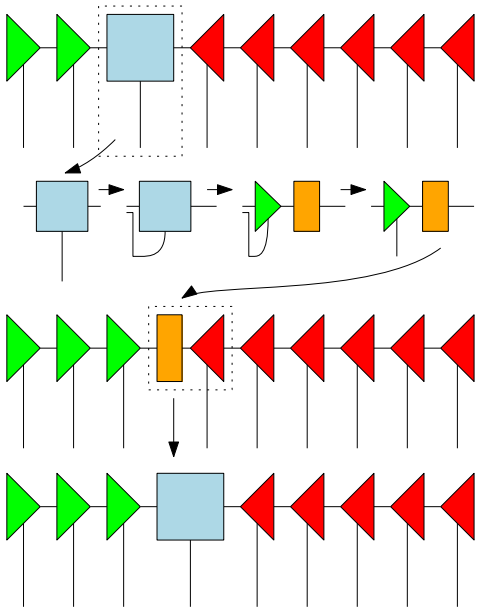

Figure 9: *Moving the orthogonality center one site to the right using the QR factorization. This can be repeated to move the orthogonality center to any site to the right of its current position. To move the orthogonality center to the left, a similar process is used substituting the LQ factorization for the QR factorization.*

Time Evolving Block Decimation

Time evolving block decimation (TEBD) is a method for efficiently simulating 1D quantum systems with low entanglement. By leveraging the fidelity of the system's MPS decomposition, a Suzuki-Trotter [3] decomposition of the propogator

$$\hat{U}(t) = \exp\{-i\hat{H}t/\hbar\}$$

can be applied step-by-step to the MPS with bond dimensions truncated after each step. For the 1-D transverse field Ising model

$$\hat{H} = \sum_{i=1}^{N-1} \sigma_z^{(i)} \sigma_z^{(i+1)} + J \sum_{i=1}^{N} \sigma_x^{(i)}$$

this amounts to applying p Trotterized operators (setting $\hbar = 1$):

$$\hat{U}(t) = \left[\left(\prod_{i=1}^{N-1} e^{-i\sigma_z^{(i)}\sigma_z^{(i+1)}\Delta t} \right) \left(\prod_{i=1}^{N} e^{-i\sigma_x^{(i)}\Delta t} \right) \right]^p$$

where the step size $\Delta t = \frac{t}{p}$. A depiction of one TEBD sweep with this Hamiltonian is shown in figure 10.

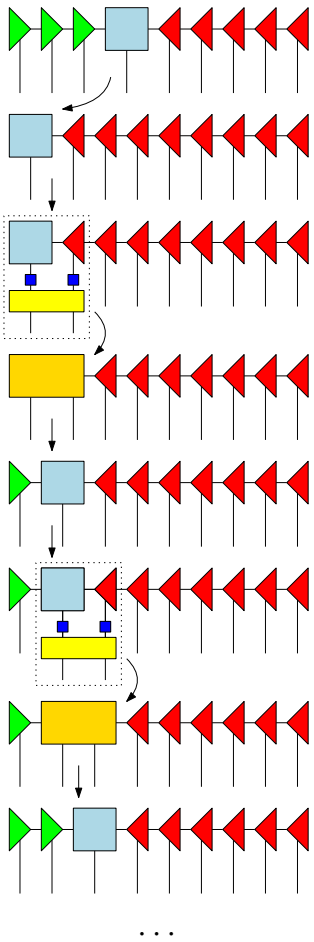

Figure 10: *One step of time evolving block decimation. The orthogonality center is moved to the leftmost site. Trotterized operators $R_x(\Delta t)$ in blue and $R_{zz}(\Delta t)$ in yellow are applied to the orthogonality center and its rightmost neighbor. A SVD is performed and the singular value matrix is truncated and contracted to the right to enforce the bond dimension χ. The sweep continues until reaching the last site, at which point the orthogonality center is again moved to the leftmost site and the above process is repeated $p-1$ additional times.*

This approximation is not sufficient when the Hamiltonian $\hat{H}$ generates sufficiently high entanglement, since enforcing the maximum bond dimension χ bounds the maximum amout of entanglement the MPS can ever reach. If, however, $\hat{H}$ consists entirely of single-site terms, then this method is exact since the systems entanglement cannot grow through time evolution under $\hat{H}$. See the rightmost heatmap in figure 12 for an example of what time evolution under a nonentangling Hamiltonian might look like.

Package Overview

This section provides an overview of the real core of this project: a Julia package for creating and manipulating matrix product states, located at `https://github.com/gl3nnleblanc/pdrp2021`.

Julia

Julia is a modern programming language incubated at MIT in 2009 and designed from the beginning with high performance in mind [4]. Julia is fast, easy to use, and open source.

Algorithms

The following section contains pseucode outlining the main ideas of what was implemented in the package. Again, the full code written in Julia is available at the repository.

Data: input tensor T, left_dim,
right_dim, χ
Result: length(Σ), T_{next}, V
$T_{MAT} \leftarrow\!\shortmid$ reshape(T, left_dim, right_dim);
T_{next}, Σ, $V^\dagger \leftarrow\!\shortmid$ SVD(T_{MAT});
$V \leftarrow\!\shortmid (V^\dagger)^\dagger$;
$\Sigma \leftarrow\!\shortmid$ truncate_to_chi(Σ, χ);
$T_{next} \leftarrow\!\shortmid$ truncate_to_chi(T_{next}, χ);
return length(Σ), T_{next}, V;

Algorithm 1: Helper function for splitting a tensor.

Data: input tensor Ψ, desired bond dimension χ
N $\leftarrow\!\shortmid$ tensor rank of Ψ;
sites $\leftarrow\!\shortmid$ [ ];
d_{next}, T_{next}, T_{curr} $\leftarrow\!\shortmid$ split_tensor(Ψ, 2^{N-1}, 2, χ);
sites.append(T_{curr});
for $i \leftarrow\!\shortmid$ *2 to* $N-1$ **do**
  d_{next}, T_{next}, T_{curr} $\leftarrow\!\shortmid$ split_tensor(T_{next}, 2^{N-i}, 2^i, χ);
  if *length*(T_{curr}) $= \chi^2$ * 2 **then**
    T_{curr} $\leftarrow\!\shortmid$ reshape(T_{curr}, χ, 2, χ);
  else
    d_{prev} $\leftarrow\!\shortmid$ length(T_curr) $\div$ $(2 \times d_{next})$;
    T_{curr} $\leftarrow\!\shortmid$ reshape(T_{curr}, d_{next}, 2, d_{prev});
  end
  sites.append(T_{curr});
end
-, T_{next}, T_{curr} $\leftarrow\!\shortmid$ split_tensor(T_{next}, 2, d_{prev}, χ);
T_{curr} $\leftarrow\!\shortmid$ reshape(T_curr, 2, 2, :);
sites.append(T_{curr});
sites.append(T_{next});
return MPS(sites, χ, N);

Algorithm 2: Generating a MPS from input tensor Ψ.

Algorithm 2 returns a MPS wrapper consisting of an array of tensors arranged from left to right in descending order. Said another way, the Nth entry of this array is the leftmost site.

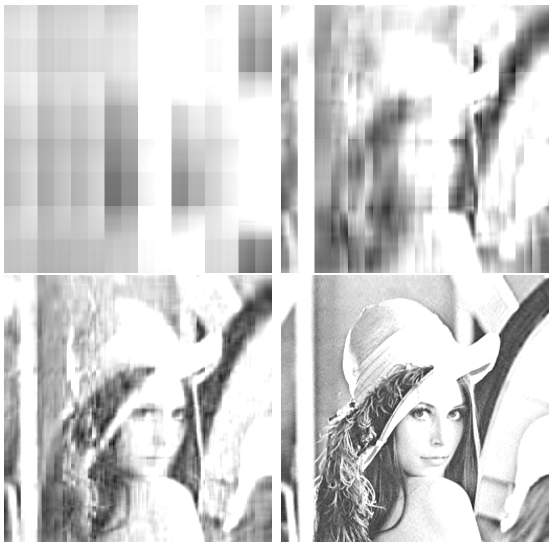

Figure 11: *Compressing an image with an MPS. Clockwise from top left:* $\chi = 2$, $\chi = 9$, $\chi = 20$, $\chi = 100$, *with compression ratios of 1927.5, 126.2, 31.3, and 2.24, respectively. Lossless storage as a MPS results in a compression ratio less than 1.*

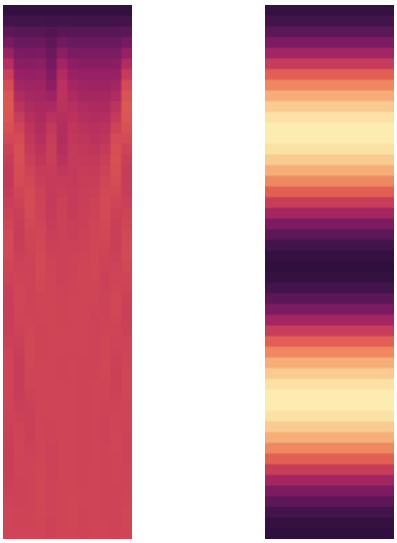

Figure 12: *Heatmaps of* $\langle\sigma_z\rangle$ *for each site in a chain of 12 qubits time evolving under a* $(J = 1)$ *1D Ising model with (left) and without (right) the local interaction term* $\sigma_z^{(i)}\sigma_z^{(i+1)}$. *Using an MPS with* $\chi = 32$ *and running 1000 sweeps on an Intel i5-6600k @ 3.9 GHz took* ≈ 3 *minutes.*

Examples

There are three example notebooks contained in the repository (as linked above). Some highlights:

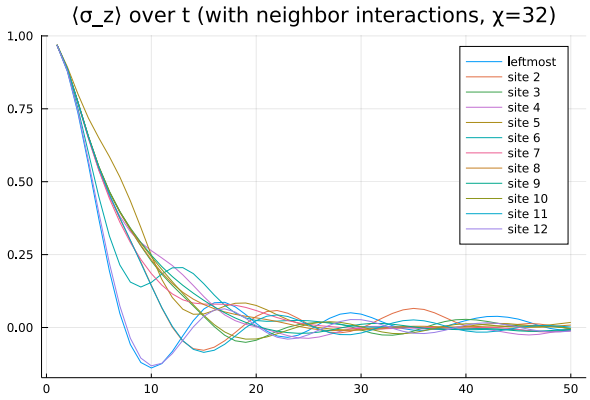

Figure 13: *Graph corresponding to the left heatmap in figure 12.*

Next Steps

This project felt extremely rewarding and I'm planning to continue sporadically adding things to it over the summer when I have the time. Two things that I'd like to implement are DMRG [5] and a neural network using a MPS whose sites correspond to lifted features [6], [7].

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