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Density matrix renormalization group method

The density matrix renormalization group, proposed in 1992 by White [1], is introduced in its historical context. To highlight the ideas that led to this method, we explain the real-space renormalization group, proposed by Wilson [2] in 1975. We then explain how the shortcomings of Wilson's method led to the density matrix renormalization group.

1.1 Introduction

Consider the problem of numerically finding the ground state $|\Psi_0\rangle$ of an N-site one-dimensional spin-$\frac{1}{2}$ system.

The underlying Hilbert space of the system is a tensor product of the local Hilbert spaces $\mathscr{H}_{\text{site}}$, which are spanned by the states $\{|\uparrow\rangle, |\downarrow\rangle\}$. Thus, a general state of the system is a unit vector in a 2^N-dimensional space

$$|\Psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots\in\{|\uparrow\rangle,|\downarrow\rangle\}} c_{\sigma_1,\sigma_2,\ldots,\sigma_N} |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \ldots \otimes |\sigma_N\rangle . \tag{1.1}$$

For a system with 1000 particles, the dimensionality of the Hilbert space comes in at about 10^{301}, some 220 orders of magnitude larger than the number of atoms in the observable universe. How can we possibly hope to approximate states in this space?

As it turns out, nature is very well described by Hamiltonians that are local – that do not contain interactions between an arbitrary number of bodies. And for these Hamiltonians, only an exponentially small subset of states can be explored in the lifetime of the universe [3]. That is, only exponentially few states are physical. The low-energy states, especially, have special properties that allow them to be very well approximated by a polynomial number

of parameters. This explains the existence of algorithms, of which the density matrix normalization group is the most widely celebrated one, that can approximate certain quantum systems to machine precision.

Refer to where this will be made more precise.

1.2 Density matrix renormalization group

The density matrix renormalization group (DMRG), introduced in 1992 by White [1], aims to find the best approximation of a many-body quantum state, given that only a fixed amount of basis vectors is kept. This amounts to finding the best truncation

$$\mathscr{H}_N \to \mathscr{H}_{\text{eff}} \tag{1.2}$$

from the full N-particle Hilbert space to an effective lower dimensional one. This corresponds to renormalizing the Hamiltonian H.

Before DMRG, several methods for achieving this truncation were proposed, most notably Wilson's real-space renormalization group [2]. We will discuss this method first, and highlight its shortcomings, which eventually led to the invention of the density-matrix renormalization group method by White.

1.2.1 Real-space renormalization group

Consider again the problem of finding the ground state of a many-body Hamiltonian H. A natural way of renormalizing H in real-space is by partitioning the lattice in blocks, and writing H as

$$H = H_A \otimes \ldots \otimes H_A \tag{1.3}$$

where H_A is the Hamiltonian of a block.

Make figures.

The real-space renormalization procedure now entails finding an effective Hamiltonian H'_A of the two-block Hamiltonian $H_{AA} = H_A \otimes H_A$. In the method introduced by Wilson, H'_A is formed by keeping the m lowest lying eigenstates $|\epsilon_i\rangle$ of H_{AA}:

$$H'_A = \sum_{i=1}^{m} \epsilon_i \, |\epsilon_i\rangle \langle\epsilon_i| \, . \tag{1.4}$$

This is equivalent to writing

$$H'_A = OH_{AA}O^\dagger, \tag{1.5}$$

with O an $m \times 2^L$ matrix, with rows being the m lowest-lying eigenvectors of H_{AA}, and L the number of lattice sites of a block. At the fixed point of this iteration procedure, H_A represents the Hamiltonian of an infinite chain. In choosing this truncation, it is assumed that the low-lying eigenstates of the system in the thermodynamic limit are composed of low-lying eigenstates of smaller blocks.

It turns out that this method gives poor results for many lattice systems. Following an example put forth by White and Noack [4], we establish an intuition why.

1.2.2 Single particle in a box

Consider the Hamiltonian

$$H = 2\sum_i |i\rangle\langle i| - \sum_{\langle i,j\rangle} |i\rangle\langle j|, \tag{1.6}$$

where the second summation is over nearest neighbors $\langle i, j\rangle$. H represents the discretized version of the particle-in-a-box Hamiltonian, so we expect its ground state to be approximately a standing wave with wavelength double the box size. However, the blocking procedure just described tries to build the ground state iteratively from ground states of smaller blocks. No matter the amount of states kept, the final result will always incur large errors.

For this simple model, White and Noack solved the problem by diagonalizing the Hamiltonian of a block with different boundary conditions, and combining the lowest eigenstates of each.

Additionally, they noted that diagonalizing $p > 2$ blocks, and projecting out $p - 2$ blocks to arrive at H_{AA} also gives accurate results, and that this is a generalization of applying multiple boundary conditions.

Figure.

In the limit $p \to \infty$ this method becomes exact, since we then find exactly the correct contribution of H_{AA} to the final ground state. It is a slightly changed version of this last method that is now known as DMRG.

1.2.3 Density matrix method

The fundamental idea of the density matrix renormalization group method rests on the fact that if we know the state of the final lattice, we can find the m most important states for H_{AA} by diagonalizing the reduced density matrix ρ_{AA} of the two blocks.

To see this, suppose, for simplicity, that the entire lattice is in a pure state[1] $|\Psi\rangle = \sum c_{b,e} |b\rangle |e\rangle$, with $b = 1, \ldots, l$ the states of H_{AA} and $e = 1, \ldots, N_{\text{env}}$ the environment states. The reduced density matrix is given by

$$\rho_{AA} = \sum_e |\Psi\rangle \langle\Psi| = \sum_{b,b'} c_{b,e} c_{b',e} |b\rangle \langle b'| \tag{1.7}$$

We now wish to find a set of orthonormal states $|\lambda\rangle \in \mathcal{H}_{AA}$, $\lambda = 1, \ldots, m$ with $m < l$, such that the quadratic norm

$$\| |\Psi\rangle - |\widetilde{\Psi}\rangle \| = 1 - 2 \sum_{\lambda,b,e} a_{\lambda,e} c_{b,e} u_{\lambda,b} + \sum_{\lambda,e} a_{\lambda,e}^2 \tag{1.8}$$

is minimized. Here,

$$|\widetilde{\Psi}\rangle = \sum_{\lambda=1}^{m} \sum_{e=1}^{N_{\text{env}}} a_{\lambda,e} |\lambda\rangle |e\rangle \tag{1.9}$$

is the representation of $|\Psi\rangle$ given the constraint that we can only use m states from $\mathcal{H}_{AA}$. The $u_{\lambda,b}$ are given by

$$\lambda = \sum_b u_{\lambda,b} |b\rangle . \tag{1.10}$$

We need to minimize (1.8) with respect to $a_{\lambda,e}$ and $u_{\lambda,b}$. Setting the derivative with respect to $a_{\lambda,e}$ equal to 0 yields

$$-2 \sum_{\lambda,b,e} c_{b,e} u_{\lambda,b} + 2 \sum_{\lambda,e} a_{\lambda,e} = 0 \tag{1.11}$$

So we see that $a_{\lambda,e} = \sum_b c_{b,e} u_{\lambda,b}$, and we are left to minimize

$$1 - \sum_{\lambda,b,b'} u_{\lambda,b} (\rho_{AA})_{b,b'} u_{\lambda,b'} \tag{1.12}$$

[1] For a proof for a mixed state, see [5]

with respect to $u_{\lambda,b}$. But this is equal to

$$1 - \sum_{\lambda=1}^{m} \langle \lambda | \, \rho_{AA} \, | \lambda \rangle \tag{1.13}$$

and because the eigenvalues of ρ_{AA} represent probabilities and are thus non-negative, this is clearly minimal when $|\lambda\rangle$ are the m eigenvectors of ρ_{AA} corresponding to the largest eigenvalues. This minimal value is

$$1 - \sum_{\lambda=1}^{m} w_\lambda \tag{1.14}$$

with w_λ the eigenvalues of the reduced density matrix.

(1.14) is called the truncation error or residual probability, and quantifies the incurred error when taking a number $m < l$ states to represent $\mathcal{H}_{AA}$.

We have proven that the optimal (in the sense that $\| \, |\Psi\rangle - |\widetilde{\Psi}\rangle \, \|$ is minimized[2]) states to keep for a subsystem are the states given by the reduced density matrix, obtained by tracing out the entire lattice in the ground state (or some other target state).

The problem, of course, is that we do not know the state of the entire lattice, since that is exactly what we're trying to approximate.

Instead then, we should try to calculate the reduced density matrix of the system embedded in *some* larger environment, as closely as possible resembling the one in which it should be embedded. The combination of the system block and this environment block is usually called *superblock*.

Analogous to how White and Noack solved the particle in a box problem, we could calculate the ground state of $p > 2$ blocks, and trace out all but 2, doubling our block size each iteration. In practice, this doesn't work well for interacting Hamiltonians, since this would involve finding the largest eigenvalue of a $N^p_{\text{block}} \times N^p_{\text{block}}$ matrix (compare this with the particle in a box Hamiltonian, which only grows linearly in the amount of lattice sites).

The widely adopted algorithm proposed by White [7] for finding the ground state of a system in the thermodynamic limit proceeds as follows.

[2] There are several other arguments for why these states are optimal, for example, they minimize the error in expectation values $\langle A \rangle$ of operators. For an overview, see [6].

1.2.4 Infinite-system method

Add figures.

Mention boundary conditions somewere

Instead of using an exponential blocking procedure (doubling or tripling the amount of effective sites in a block at each iteration), the infinite-system method in the DMRG formulation adds a single site before truncating the Hilbert space to have at most m basis states.

1. Consider a block A of size l, with l small. Suppose, for simplicity, that the number of basis states of the block is already m. States of this block can be written as

$$|\Psi_A\rangle = \sum_{b=1}^{m} c_i \, |b\rangle \, . \tag{1.15}$$

   The Hamiltonian is written as (similarly for other operators):

$$\hat{H}_A = \sum_{b,b'}^{m} H_{bb'} \, |b\rangle \, \langle b| \, . \tag{1.16}$$

2. Construct an enlarged block with one additional site, denoted by $A\cdot$. States are now written

$$|\Psi_{A\cdot}\rangle = \sum_{b,\sigma} c_{b,\sigma} \, |b\rangle \otimes |\sigma\rangle \, . \tag{1.17}$$

   Here, σ runs over the d local basis states of $\mathscr{H}_{\text{site}}$.

3. Construct a superblock, consisting of the enlarged system block $A\cdot$ and a reflected environment block $\cdot A$, together denoted by $A\cdot\cdot A$. Find the ground state $|\Psi_0\rangle$ of $A\cdot\cdot A$, for example with the Lanczos method [8].

4. Obtain the reduced density matrix of the enlarged block by tracing out the environment, and write it in diagonal form.

$$\begin{aligned} \rho_{A\cdot} &= \sum_{e,\sigma} (\langle\sigma| \otimes \langle e|) \, |\Psi_0\rangle \, \langle\Psi_0| \, (|\sigma\rangle \otimes |e\rangle), \\ &= \sum_{i=1}^{dm} w_i \, |\lambda_i\rangle \, \langle\lambda_i| \, . \end{aligned} \tag{1.18}$$

Here, we have chosen $w_0 >= w_1 \ldots >= w_{dm}$. In this basis, the Hamiltonian is written as

$$\hat{H}_{A\cdot} = \sum_{i,j}^{dm} H_{ij} \left|\lambda_i\right\rangle \left\langle\lambda_j\right| . \tag{1.19}$$

5. Truncate the Hilbert space by keeping only the m eigenstates of $\rho_{A\cdot}$ with largest eigenvalues. Operators truncate as follows:

$$\widetilde{\rho}_{A\cdot} = \sum_{i=1}^{m} w_i \left|\lambda_i\right\rangle \left\langle\lambda_j\right| , \tag{1.20}$$

$$\widetilde{H}_{A\cdot} = \sum_{i,j}^{m} H_{ij} \left|\lambda_i\right\rangle \left\langle\lambda_j\right| . \tag{1.21}$$

6. Set $H_A \leftarrow \widetilde{H}_{A\cdot}$ and return to 1.

Expand. Present or link to some results. Finite-system algorithm. Maybe in other chapter: rephrase in MPS, validity of approximation: primer on entropy and eigenvalue spectrum of density matrix.

This methods finds ground state energies with astounding accuracy, and has been the reference point in all 1D quantum lattice simulation since its invention.

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