Contents

Chapter 1

Introduction

1.1 Strongly interacting 1D quantum lattice models

1.1.1 The Hilbert space is enormous

Consider the problem of numerically finding the ground state $|\Psi_0\rangle$ of the N-site 1-dimensional transverse-field Ising-model, given by

$$H = -J \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^{N} \sigma_i^x \tag{1.1}$$

The underlying Hilbert space of the system is a tensor product of the local Hilbert spaces $\mathcal{H}_{\text{site}}$, 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.

$$|\Psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots \in \{|\uparrow\rangle,|\downarrow\rangle\}} c_{\sigma_1,\sigma_2,\ldots,\sigma_N} |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \ldots \otimes |\sigma_N\rangle \tag{1.2}$$

So, 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. 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 [7]. That is, only exponentially few states are physical.

Expand a bit. Refer back to problem of finding ground state.

Chapter 2

Density matrix renormalization group method

2.1 Abstract

The variational method is introduced in its historical context – that of interacting 1D quantum lattice systems. An overview of White's density matrix renormalization group [9] is given. Then, the formal connection to 2D classical lattices is made.

2.2 Density matrix renormalization group

The density matrix renormalization group (DMRG), introduced in 1992 by White [9], 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

$$\mathcal{H}_N \to \mathcal{H}_{\text{eff}} \tag{2.1}$$

From the full N-particle Hilbert space to an effective lower dimensional one. This corresponds to renormalizing the Hamiltonian H. Before the DMRG paper, several methods for achieving this truncation were proposed, most notably Wilson's real-space renormalization group [12].

2.2.1 Real-space renormalization group

Consider 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

$$H = H_A \otimes \ldots \otimes H_A \tag{2.2}$$

where H_A is the Hamiltonian of a block.

Make figures.

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

$$H'_A = \sum_{i=1}^{m} \epsilon_i \, |\epsilon_i\rangle \langle\epsilon_i| \tag{2.3}$$

This is equivalent to writing

$$H'_A = O H_{AA} O^\dagger \tag{2.4}$$

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.

Explain renormalization group idea somewhere.

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 [11], we establish here an intuition why.

2.2.2 Single particle in a box

Consider the Hamiltonian

$$H = 2 \sum_i |i\rangle \langle i| - \sum_{\langle i,j \rangle} |i\rangle \langle j| \tag{2.5}$$

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. 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.

2.2.3 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

$$\rho_{AA} = \sum_{e} |\Psi\rangle \langle\Psi| = \sum_{b,b'} c_{b,e} c_{b',e} |b\rangle \langle b'| \tag{2.6}$$

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

$$\| |\Psi\rangle - |\widetilde{\Psi}\rangle \| = 1 - 2 \sum_{\lambda,b,e} a_{\lambda,e} c_{b,e} u_{\lambda,b} + \sum_{\lambda,e} a_{\lambda,e}^2 \tag{2.7}$$

[1] For a proof for a mixed state, see [6]

is minimized. Here,

$$|\widetilde{\Psi}\rangle = \sum_{\lambda=1}^{m} \sum_{e=1}^{N_{\text{env}}} a_{\lambda,e} \, |\lambda\rangle \, |e\rangle \tag{2.8}$$

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

$$\lambda = \sum_{b} u_{\lambda,b} \, |b\rangle \tag{2.9}$$

We need to minimize (2.7) with respect to $a_{\lambda,e}$ and $u_{\lambda,b}$. Setting the derivative with respect to $a_{\lambda,e}$ equal to 0 yields

$$-2 \sum_{\lambda,b,e} c_{b,e} u_{\lambda,b} + 2 \sum_{\lambda,e} a_{\lambda,e} = 0 \tag{2.10}$$

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

$$1 - \sum_{\lambda,b,b'} u_{\lambda,b} (\rho_{AA})_{b,b'} u_{\lambda,b'} \tag{2.11}$$

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

$$1 - \sum_{\lambda=1}^{m} \langle\lambda| \, \rho_{AA} \, |\lambda\rangle \tag{2.12}$$

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

$$1 - \sum_{\lambda=1}^{m} w_\lambda \tag{2.13}$$

with w_λ the eigenvalues of the reduced density matrix. (2.13) is called the truncation error or residual probability, and quantifies the incurred error when taking a number $m < l$ states to represent $\mathcal{H}_{AA}$.

Look ahead to SVD

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 [10] for finding the ground state of a system in the thermodynamic limit proceeds as follows.

2.2.4 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

$$|\Psi_A\rangle = \sum_{b=1}^{m} c_i |b\rangle \tag{2.14}$$

[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 [8].

The Hamiltonian is written as (similarly for other operators)

$$\hat{H}_A = \sum_{b,b'}^{m} H_{bb'} \left|b\right\rangle \left\langle b\right| \tag{2.15}$$

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

$$\left|\Psi_{A\cdot}\right\rangle = \sum_{b,\sigma} c_{b,\sigma} \left|b\right\rangle \otimes \left|\sigma\right\rangle \tag{2.16}$$

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

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 $\left|\Psi_0\right\rangle$ of $A\cdot\cdot A$, for example with the Lanczos method.

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

$$\begin{aligned} \rho_{A\cdot} &= \sum_{e,\sigma} (\left\langle\sigma\right| \otimes \left\langle e\right|) \left|\Psi_0\right\rangle \left\langle\Psi_0\right| (\left|\sigma\right\rangle \otimes \left|e\right\rangle) \\ &= \sum_{i=1}^{dm} w_i \left|\lambda_i\right\rangle \left\langle\lambda_i\right| \end{aligned} \tag{2.17}$$

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

$$\hat{H}_{A\cdot} = \sum_{i,j}^{dm} H_{ij} \left|\lambda_i\right\rangle \left\langle\lambda_j\right| \tag{2.18}$$

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

$$\widetilde{\rho}_{A\cdot} = \sum_{i=1}^{m} w_i \left|\lambda_i\right\rangle \left\langle\lambda_j\right| \tag{2.19}$$

$$\widetilde{H}_{A\cdot} = \sum_{i,j}^{m} H_{ij} \left|\lambda_i\right\rangle \left\langle\lambda_j\right| \tag{2.20}$$

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, 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.

Chapter 3

DRMG applied to 2D classical lattice models

3.1 Partition functions of classical lattices

The central quantity in equilibrium statistical mechanics is the partition function Z, which, for a discrete system such as a lattice, is defined as

$$Z = \sum_s \exp\left(-\beta H(s)\right) \tag{3.1}$$

where the sum is over all microstates s, H is the energy function, and $\beta = T^{-1}$ the inverse temperature.

3.2 Transfer matrices of lattice models

3.2.1 1D Ising model

refer to Ising, talk a bit about model (magnetism etc).

Consider the 1D zero-field ferromagnetic Ising model, defined by the energy function

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{3.2}$$

Here, we sum over nearest neighbors $\langle ij \rangle$ and the spins σ_i take the values ± 1. $J > 0$. Assume, for the moment, that the chain consists of N spins, and apply periodic boundary conditions. The partition function of this system is given by

$$Z_N = \sum_{\sigma_1,\ldots,\sigma_N \in \{-1,1\}} \exp(-\beta H(\sigma)) \tag{3.3}$$

Exploiting the local nature of the interaction between spins, we can write

$$Z_N = \sum_{\sigma_1,\cdots,\sigma_N \in \{-1,1\}} \prod_{\langle i,j \rangle} e^{K\sigma_i\sigma_j} \tag{3.4}$$

where we defined $K \equiv \beta J$. Now, we can define the 2×2 matrix $T_{\sigma\sigma'} = \exp(K\sigma\sigma')$ to get

$$Z_N = \sum_{\sigma_1,\cdots,\sigma_N} T_{\sigma_1\sigma_2} \cdots T_{\sigma_N\sigma_1} = \operatorname{Tr} T^N \tag{3.5}$$

T is called the transfer matrix. Since $T^N = PD^NP^{-1}$, where P consists of the eigenvectors of T, and by the cyclic property of the trace, we have

$$Z_N = \lambda_1^N + \lambda_2^N \tag{3.6}$$

Thus, we have reduced the problem of finding the partition function to an eigenvalue problem, which is quite easy in this case. Also, note that in the thermodynamic limit $N \to \infty$

$$Z = \lim_{N\to\infty} \lambda_1^N \tag{3.7}$$

where λ_1 is the non-degenerate largest eigenvalue (in absolute value) of T.

3.2.2 2D Ising model

Talk about exact solution (Onsager). Why is it important? Maybe star-triangle relation (Baxter). Not all IRF models solvable.

Next, we treat the two-dimensional, square-lattice Ising model. In two dimensions, the energy function is still written as in (3.2), but now every lattice site has four neighbors. Let N be the number of columns

and l be the number of rows of the lattice, and assume $l \gg N$. In the vertical direction, we apply periodic boundary conditions, as in the one-dimensional case. In the horizontal direction, we keep an open boundary. We refer to N as the system size.
Similarly to the 1D case, the partition function can be written as

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{\langle i,j,k,l \rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{3.8}$$

where the product runs over all groups of four spins sharing the same face. The Boltzmann weight of such a face is given by

$$W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = \exp\left\{ \frac{K}{2} (\sigma_i\sigma_j + \sigma_j\sigma_k + \sigma_k\sigma_l + \sigma_l\sigma_i) \right\} \tag{3.9}$$

We can express the Boltzmann weight of a configuration of the whole lattice as a product of the Boltzmann weights of the rows

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{r=1}^{l} W(\sigma_1^r, \sigma_2^r, \sigma_1^{r+1}, \sigma_2^{r+1}) \dots W(\sigma_{N-1}^r, \sigma_N^r, \sigma_{N-1}^{r+1}, \sigma_N^{r+1}) \tag{3.10}$$

Where σ_i^r denotes the value of the ith spin of row r. Now, we can generalize the definition of the transfer matrix to two dimensions, by defining it as the Boltzmann weight of an entire row

$$T_N(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) = W(\sigma_1, \sigma_2, \sigma_1', \sigma_2') \dots W(\sigma_{N-1}, \sigma_N, \sigma_{N-1}', \sigma_N') \tag{3.11}$$

The dimensions of T_N are $2^N \times 2^N$. Similarly as in the one-dimensional case, the partition function now becomes

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{r=1}^{l} T_N(\boldsymbol{\sigma}^r, \boldsymbol{\sigma}^{r+1}) = \operatorname{Tr} T_N^l \tag{3.12}$$

In the limit of an $N \times \infty$ cylinder, the partition function is once again determined by the largest eigenvalue.

$$Z_N = \lim_{l\to\infty} T_N^l = \lim_{l\to\infty} (\lambda_0)_N^l \tag{3.13}$$

The partition function in the thermodynamic limit is given by

$$Z = \lim_{N\to\infty} Z_N \tag{3.14}$$

3.3 Partition function of 2D lattice as a tensor network

In calculating the partition function of 1D and 2D lattices, matrices of Boltzmann weights like W and T play a crucial role. Up until now, we have formulated them in a way that serves us analytically, but makes it less clear how we should use them to implement a partition sum in a computer program, when calculations typically have to be written as matrix multiplications in order to be fast. Now, we rewrite the partition sum of 2D classical lattices in the language of tensor networks to make the computational steps more manifest, while retaining the intuitions of the earlier formulation.

3.4 Transfer matrix renormalization group

More about connection between 1D quantum and 2D classical

Pictures

Nishino [4] was the first one to apply DMRG in its modern form to approximate the transfer matrix of a two-dimensional classical lattice system.
In the limit of an $N \times \infty$ lattice, T_N^l becomes proportional to the projector onto the eigenspace of the largest eigenvalue

$$\lim_{l\to\infty} T_N^l = \lim_{l\to\infty} (\lambda_0)_N^l \left|\lambda_0\right\rangle_N \left\langle\lambda_0\right|_N \sim \left|\lambda_0\right\rangle_N \left\langle\lambda_0\right|_N \tag{3.15}$$

Now, the connection to ground state DMRG is clear. Recall the full-system density matrix of an N-site 1D quantum lattice system (the superblock) in the ground state (cf. (2.6))

$$\rho_N = \left|\Psi_0\right\rangle_N \left\langle\Psi_0\right|_N \tag{3.16}$$

Write down equations that are analogous to reduced density matrix.
Pictures

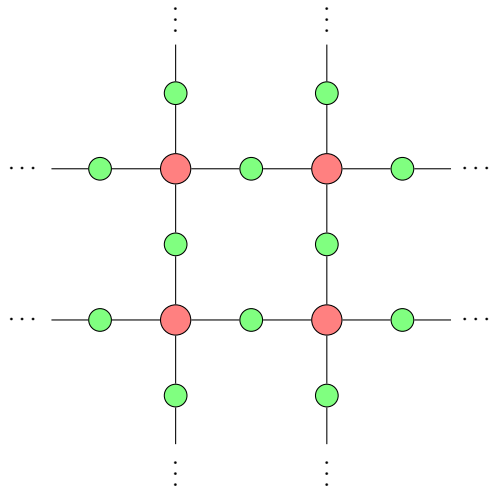

Figure 3.1: 2D lattice to as a tensor network. bla bla.

3.5 Corner transfer matrices

The concept of corner transfer matrices for 2D lattices was first introduced by Baxter [1, 2, 3]. Whereas the row-to-row transfer matrix (3.11) corresponds to adding a row to the lattice, the corner transfer matrix adds a quadrant of spins. It is defined as

$$A_{\boldsymbol{\sigma},\boldsymbol{\sigma'}} = \begin{cases} \sum \prod_{\langle i,j,k,l \rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) & \text{if } \sigma_1 = \sigma_1' \\ 0 & \text{if } \sigma_1 \neq \sigma_1' \end{cases} \tag{3.17}$$

Picture.

Here, the product runs over groups of four spins that share the same face, and the sum is over all spins in the interior of the quadrant. In a symmetric and isotropic model, we have

$$W(a,b,c,d) = W(b,a,d,c) = W(c,a,d,b) = W(d,c,b,a) \tag{3.18}$$

and the partition of an $N \times N$ lattice is expressed as

$$Z_{N\times N} = \operatorname{Tr} A^4 \tag{3.19}$$

In the thermodynamic limit, (3.19) is equal to (3.12).

3.5.1 Corner transfer matrix renormalization group

More about Baxter's variational approach.

Nishino and Okunishi combined ideas from Baxter and White to formulate the corner transfer matrix renormalization group [5].

Chapter 4

Matrix Product States

4.1 From the DMRG algorithm to matrix product states

Appendix A

Correspondence of 1D quantum and 2D classical lattices

A.1 Hoi

lorem hallo

Appendix B

Introduction to tensor networks

B.1 Tensors, or multidimensional arrays

In the field of tensor networks, a tensor is a multidimensional table with numbers – a convenient way to organize information. It is the generalization of a vector

$$v_i = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} \tag{B.1}$$

which has one index, and a matrix

$$M_{ij} = \begin{bmatrix} M_{11} & \dots & M_{1n} \\ \vdots & & \vdots \\ M_{m1} & \dots & M_{mn} \end{bmatrix} \tag{B.2}$$

which has two. A tensor of rank N has N indices[1]

$$T_{i_1 \dots i_N} \tag{B.3}$$

[1] The definition of rank in this context is not to be confused with the rank of a matrix, which is the number of linearly independent columns. Synonyms of tensor rank are tensor degree and tensor order.

B.2 Tensor contraction

Tensor contraction is the higher-dimensional generalization of the dot product

$$\boldsymbol{a} \cdot \boldsymbol{b} = \sum_i a_i b_i \tag{B.4}$$

where a lower-dimensional tensor (in this case, a scalar, which is a zero-dimensional tensor) is obtained by summing over all values of a repeated index. Examples are matrix-vector multiplication

$$(M\boldsymbol{a})_i = \sum_j M_{ij} a_j \tag{B.5}$$

and matrix-matrix multiplication

$$(AB)_{ij} = \sum_k A_{ik} B_{kj} \tag{B.6}$$

But a more elaborate tensor multiplication could look like

$$w_{abc} = \sum_{d,e,f} T_{abcdef} v_{def} \tag{B.7}$$

As with the dot product between vectors, matrix-vector multiplication and matrix-matrix multiplication, a contraction between tensors is only defined if the dimensions of the indices match.

B.3 Tensor networks

A tensor network is specified by a set of tensors, together with a set of contractions to be performed. For example:

$$M_{ab} = \sum_{i,j,k} A_{ai} B_{ij} C_{jk} D_{kb} \tag{B.8}$$

which corresponds to the matrix product $ABCD$.

B.3.1 Graphical notation

It is highly convenient to introduce a graphical notation, which greatly simplifies expressions and makes certain properties manifest.

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