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DRMG applied to two-dimensional classical lattice models

1.1 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

$$Z = \sum_s \exp\left(-\beta H(s)\right) \tag{1.1}$$

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

1.2 Transfer matrices of lattice models

1.2.1 1D Ising model

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

Consider the 1D zero-field ferromagnetic Ising model [4], defined by the energy function

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{1.2}$$

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

$$Z_N = \sum_{\sigma_1,\ldots,\sigma_N \in \{-1,1\}} \exp(-\beta H(\sigma)) \tag{1.3}$$

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

$$Z_N = \sum_{\sigma_1,\cdots,\sigma_N \in \{-1,1\}} \prod_{\langle i,j \rangle} e^{K\sigma_i\sigma_j} \tag{1.4}$$

where we defined $K \equiv \beta J$.

Now, we define the 2×2 matrix

$$T_{\sigma\sigma'} = \exp(K\sigma\sigma') \tag{1.5}$$

A possible choice of basis is

$$(|\uparrow\rangle = 1, |\downarrow\rangle = -1) = (\begin{bmatrix}1\\0\end{bmatrix}, \begin{bmatrix}0\\1\end{bmatrix}) \tag{1.6}$$

In terms of this matrix, Z_N is written as

$$Z_N = \sum_{\sigma_1,\cdots,\sigma_N} T_{\sigma_1\sigma_2} \cdots T_{\sigma_N\sigma_1} = \mathrm{Tr}\, T^N \tag{1.7}$$

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

$$Z_N = \lambda_1^N + \lambda_2^N \tag{1.8}$$

Thus, we have reduced the problem of finding the partition function to an eigenvalue problem, which is quite easy in this case.

Note that in the thermodynamic limit $N \to \infty$

$$Z = \lim_{N\to\infty} \lambda_1^N \tag{1.9}$$

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

Fixed boundary conditions

We may also apply fixed boundary conditions. The partition function is then written as

$$Z_N = \langle \sigma' | \, T^N \, | \sigma \rangle \,, \tag{1.10}$$

where $|\sigma\rangle$ and $|\sigma'\rangle$ are the right and left boundary spins.

In the large-N limit, T^N tends towards the projector onto the eigenspace spanned by the eigenvector belonging to the largest eigenvalue

$$|\lambda_1\rangle = \lim_{N\to\infty} \frac{T^N \, |\sigma\rangle}{\left\| T^N \, |\sigma\rangle \right\|}. \tag{1.11}$$

Equation 1.11 is true for any $|\sigma\rangle$ that is not orthogonal to $|\lambda_1\rangle$.

The physical significance of the normalized lowest-lying eigenvector $|\lambda_1\rangle$ is that $\langle\lambda_1|\uparrow\rangle$ and $\langle\lambda_1|\downarrow\rangle$ represent the Boltzmann weight of $|\uparrow\rangle$ and $|\downarrow\rangle$ at the boundary of a half-infinite chain.

1.2.2 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 Equation 1.2, 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 as in the 1D case, the partition function can be written as

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{\langle i,j,k,l \rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{1.12}$$

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

$$W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = \exp\left\{ \frac{K}{2} (\sigma_i\sigma_j + \sigma_j\sigma_k + \sigma_k\sigma_l + \sigma_l\sigma_i) \right\} \tag{1.13}$$

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

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{r=1}^{l} W(\sigma_1^r, \sigma_2^r, \sigma_1^{r+1}, \sigma_2^{r+1}) \ldots W(\sigma_{N-1}^r, \sigma_N^r, \sigma_{N-1}^{r+1}, \sigma_N^{r+1}) \quad (1.14)$$

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

$$T_N(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) = W(\sigma_1, \sigma_2, \sigma_1', \sigma_2') \ldots W(\sigma_{N-1}, \sigma_N, \sigma_{N-1}', \sigma_N') \quad (1.15)$$

If we take the spin configurations of an entire row as basis vectors, T_N can be written as a matrix of dimensions $2^N \times 2^N$.

Similarly as in the one-dimensional case, the partition function now becomes

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{r=1}^{l} T_N(\boldsymbol{\sigma}^r, \boldsymbol{\sigma}^{r+1}) = \mathrm{Tr}\, T_N^l \quad (1.16)$$

In the limit of an $N \times \infty$ cylinder, the partition function is once again determined by the largest eigenvalue[1].

$$Z_N = \lim_{l\to\infty} T_N^l = \lim_{l\to\infty} (\lambda_0)_N^l \quad (1.17)$$

The partition function in the thermodynamic limit is given by

$$Z = \lim_{N\to\infty} Z_N \quad (1.18)$$

1.3 Partition function of the 2D Ising model 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. We have formulated them in a way that is valid for any interaction-round-a-face (IRF) model, defined by

$$H \sim \sum_{\langle i,j,k,l \rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \quad (1.19)$$

[1] As in the 1D case, T is symmetric, so it is orthogonally diagonalizable.

where the summation is over all spins sharing a face. W can contain 4-spin, 3-spin, 2-spin and 1-spin interaction terms. The Ising model is a special case of the IRF model, with W given by Equation 1.13.

We will now express the partition function of the 2D Ising model as a tensor network. The transfer matrix T is redefined in the process. This allows us to visualize the equations in a way that is consistent with the many other tensor network algorithms under research today.

For any l, the trace over the transfer matrix is the same in both definitions of T. It is symmetric, so they should be related by a basis transformation. Is it, perhaps, exactly the basis in which the CTM is diagonal?

1.3.1 A system of four spins

We define

$$Q(\sigma_i, \sigma_j) = \exp(K\sigma_i\sigma_j) \tag{1.20}$$

as the Boltzmann weight of the bond between σ_i and σ_j. It is the same as the 1D transfer matrix in Equation 1.5.

The Boltzmann weight of a face W decomposes into a product of Boltzmann weights of bonds

$$W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = Q(\sigma_i, \sigma_j)Q(\sigma_j, \sigma_l)Q(\sigma_l, \sigma_k)Q(\sigma_k, \sigma_i) \tag{1.21}$$

It is now easy to see that the partition function is equal to the contracted tensor network in Figure 1.1:

$$\begin{aligned} Z_{2\times 2} &= \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} \sum_{a,b,c,d} \delta_{\sigma_1,a}Q(a,b)\delta_{\sigma_2,b}Q(b,c)\delta_{\sigma_3,c}Q(c,d)\delta_{\sigma_4,d}Q(d,a) \\ &= \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} W(\sigma_1,\sigma_2,\sigma_3,\sigma_4) \end{aligned} \tag{1.22}$$

where the Kronecker delta is defined as usual:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{1.23}$$

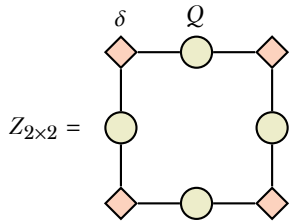

Figure 1.1: A tensor network representation of the partition function of the Ising model on a 2×2 lattice. See Equation 1.22.

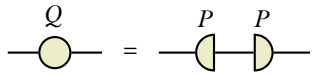

Figure 1.2: Graphical form of Equation 1.24.

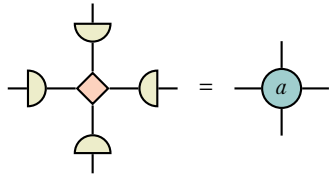

Figure 1.3: Graphical form of Equation 1.25.

1.3.2 Thermodynamic limit

We define the matrix P by

$$P^2 = Q \tag{1.24}$$

as in Figure 1.2. This allows us to write the partition function of an arbitrary $N \times l$ square lattice as a tensor network of a single recurrent tensor a_{ijkl}, given by

$$a_{ijkl} = \sum_{a,b,c,d} \delta_{abcd} P_{ia} P_{jb} P_{kc} P_{ld} \tag{1.25}$$

where the generalization of the Kronecker delta is defined as

$$\delta_{i_1 \ldots i_n} = \begin{cases} 1 & \text{if } i_1 = \ldots = i_n \\ 0 & \text{otherwise} \end{cases} \tag{1.26}$$

See Figure 1.3 and Figure 1.4. At the edges and corners, we define suitable tensors of rank 3 and 2, which we will also denote by a.

$$a_{ijk} = \sum_{abc} \delta_{abc} P_{ia} P_{jb} P_{kc}$$

$$a_{ij} = \sum_{ab} \delta_{ab} P_{ia} P_{jb}$$

The challenge is to approximate this tensor network in the thermodynamic limit.

1.3.3 The transfer matrix as a tensor network

Say something about reshaping legs.

With our newfound representation of the partition function as a tensor network, we can redefine the row-to-row transfer matrix from Equation 1.15 as the tensor network expressed in Figure 1.5. For all l, it is still true that

$$Z_{N \times l} = \operatorname{Tr} T_N^l = \sum_{i=1}^{2^N} \lambda_i^l \tag{1.27}$$

so the eigenvalues must be the same. That means that the new definition of the transfer matrix is related to the old one by a basis transformation

$$T_{\text{new}} = P T_{\text{old}} P^{-1} \tag{1.28}$$

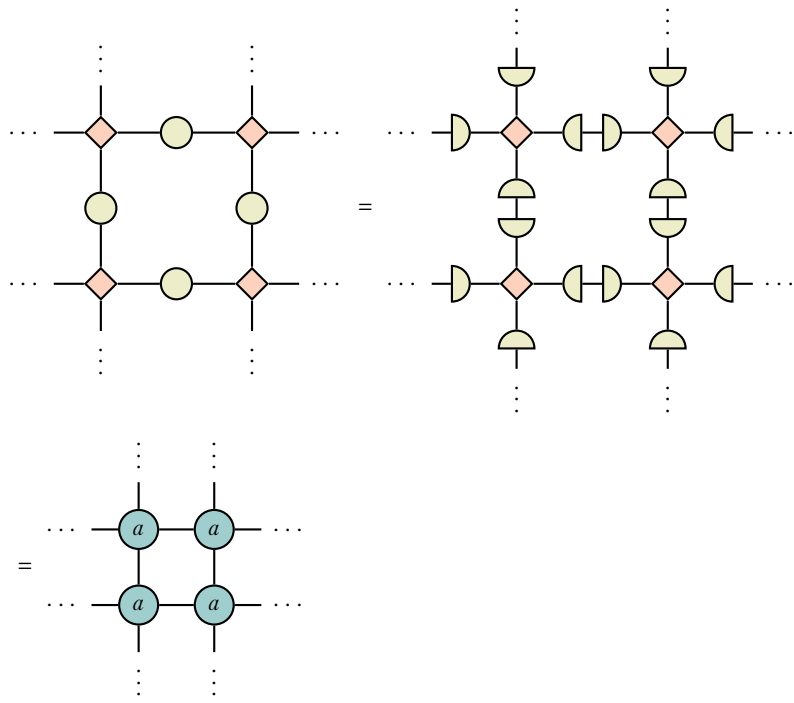

Figure 1.4: $Z_{N\times l}$ can be written as a contracted tensor network of $N \times l$ copies of the tensor a.

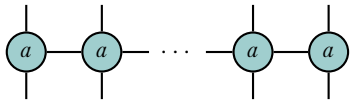

Figure 1.5: The definition of T_N as a network of N copies of the tensor a.

1.4 Transfer matrix renormalization group

There is a deep connection between quantum mechanical lattice systems in d dimensions and classical lattice systems in $d+1$ dimensions. Via the imaginary time path integral formulation, the partition function of a one-dimensional quantum system can be written as the partition function of an effective two-dimensional classical system. The ground state of the quantum system corresponds to the largest eigenvector of the transfer matrix of the classical system.

For more on the quantum-classical correspondence, see ??.

I want to refer to Baxter's variational approach anno 1968 somehwere.

Nishino [5, 6] was the first to apply density matrix renormalization group methods in the context of two-dimensional classical lattices.

1.4.1 The infinite system algorithm for the transfer matrix

Analogous to the infinite system DMRG algorithm for quantum spin chains, our goal is to approximate the transfer matrix in the thermodynamic limit as well as possible within a restriced number of basis states m. We will do this by adding a single site at a time, and truncating the dimension from $2m$ to m at each iteration.

We start the algorithm from a transfer matrix that already has dimension m, perhaps by exactly diagonalizing the transfer matrix of a couple of sites. We call this transfer matrix P_N. FIGURE.

We enlarge the system with one site by contracting with an additional a-tensor, obtaining P_{N+1}. FIGURE

In order to find the best projection from $2m$ basis states back to m, we embed the system in an environment that is the mirror image of the system

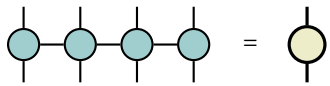

Figure 1.6: lalalala nog niks

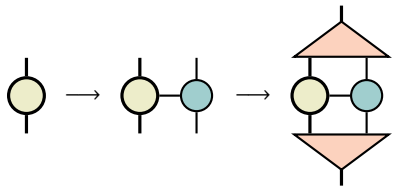

Figure 1.7: lalalala nog niks

we presently have. We call this matrix T_{2N+2}. It represents the transfer matrix of $2N+2$ sites. We find the largest eigenvalue and corresponding eigenvector, as shown in FIGURE.

Having identified the lowest-lying eigenvector of the transfer matrix with the ground state of a superblock in DMRG, the equivalent of the *reduced density matrix of a block* in the classical case is:

$$\rho_{N+1} = \sum_{\sigma_B} \langle \sigma_B | \lambda_0 \rangle \langle \lambda_0 | \sigma_B \rangle \tag{1.29}$$

where we have summed over all the degrees of freedom of one of the half-row transfer matrices P_{N+1}. FIGURE. The optimal renormalization

$$\widetilde{P}_{N+1} = O P_{N+1} O^\dagger \tag{1.30}$$

is obtained by diagonalizing ρ_{N+1} and keeping the eigenvectors corresponding to the m largest eigenvalues. FIGURE. With this blocking procedure, we can successively find

$$P_{N+1} \to P_{N+2} \to \dots \tag{1.31}$$

until we have reached some termination procedure.

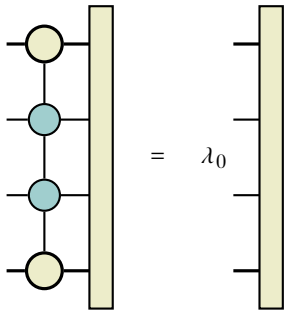

Figure 1.8: lalalala nog niks

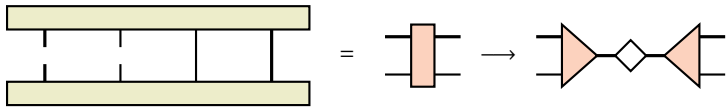

Figure 1.9: lalalala nog niks

1.5 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 (1.15) corresponds to adding a row to the lattice, the corner transfer matrix adds a quadrant of spins. It is defined as

$$A_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} = \begin{cases} \sum \prod_{\langle i,j,k,l \rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) & \text{if } \sigma_1 = \sigma_1' \\ 0 & \text{if } \sigma_1 \neq \sigma_1' \end{cases} \tag{1.32}$$

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

$$W(a,b,c,d) = W(b,a,d,c) = W(c,a,d,b) = W(d,c,b,a) \tag{1.33}$$

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

$$Z_{N\times N} = \mathrm{Tr} A^4 \tag{1.34}$$

In the thermodynamic limit, (1.34) is equal to (1.16).

1.5.1 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 [6].

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