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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, 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 can define the 2×2 matrix

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

to obtain

$$Z_N = \sum_{\sigma_1,\cdots,\sigma_N} T_{\sigma_1\sigma_2} \cdots T_{\sigma_N\sigma_1} = \mathrm{Tr}\, T^N \tag{1.6}$$

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

$$Z_N = \lambda_1^N + \lambda_2^N \tag{1.7}$$

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 $N \to \infty$

$$Z = \lim_{N\to\infty} \lambda_1^N \tag{1.8}$$

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

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 (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 to the 1D case, the partition function can be written as

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{\langle i,j,k,l \rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{1.9}$$

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

$$W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = \exp\left\{\frac{K}{2}(\sigma_i\sigma_j + \sigma_j\sigma_k + \sigma_k\sigma_l + \sigma_l\sigma_i)\right\} \tag{1.10}$$

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

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{r=1}^{l} W(\sigma_1^r, \sigma_2^r, \sigma_1^{r+1}, \sigma_2^{r+1}) \ldots W(\sigma_{N-1}^r, \sigma_N^r, \sigma_{N-1}^{r+1}, \sigma_N^{r+1}) \tag{1.11}$$

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

$$T_N(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) = W(\sigma_1, \sigma_2, \sigma_1', \sigma_2') \ldots W(\sigma_{N-1}, \sigma_N, \sigma_{N-1}', \sigma_N') \tag{1.12}$$

The dimensions of T_N are $2^N \times 2^N$.

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

$$Z_N = \sum_{\boldsymbol{\sigma}} \prod_{r=1}^{l} T_N(\boldsymbol{\sigma}^r, \boldsymbol{\sigma}^{r+1}) = \operatorname{Tr} T_N^l \tag{1.13}$$

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

$$Z_N = \lim_{l\to\infty} T_N^l = \lim_{l\to\infty} (\lambda_0)_N^l \tag{1.14}$$

The partition function in the thermodynamic limit is given by

$$Z = \lim_{N\to\infty} Z_N \tag{1.15}$$

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

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

$$H \sim \sum_{\langle i,j,k,l \rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \tag{1.16}$$

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 1.10.

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.

Help! I don't know what the formal connection between the transfer matrix and the tensor network representation is! Yes you do! 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

$$Q(\sigma_i, \sigma_j) = \exp(K\sigma_i\sigma_j) \tag{1.17}$$

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

$$W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = Q(\sigma_i, \sigma_j)Q(\sigma_j, \sigma_l)Q(\sigma_l, \sigma_k)Q(\sigma_k, \sigma_i) \tag{1.18}$$

It is now easy to see that the partition function is equal to the contracted

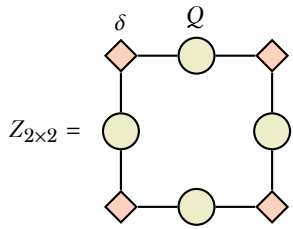

Figure 1.1: Hallo hier staat nog niks

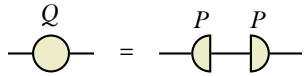

Figure 1.2: Hallo hier staat nog niks

tensor network in Figure 1.1

$$\begin{aligned} Z_{2\times 2} &= \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} \sum_{a,b,c,d} \delta_{\sigma_1,a} Q(a,b) \delta_{\sigma_2,b} Q(b,c) \delta_{\sigma_3,c} Q(c,d) \delta_{\sigma_4,d} Q(d,a) \\ &= \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} W(\sigma_1,\sigma_2,\sigma_3,\sigma_4) \end{aligned} \tag{1.19}$$

where the Kronecker delta is defined as usual:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{1.20}$$

1.3.2 Thermodynamic limit

We define the matrix P by

$$P^2 = Q \tag{1.21}$$

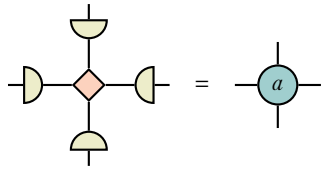

Figure 1.3: Hallo hier staat nog niks

and can now write the partition function of an arbitrary square lattice as a tensor network of a single recurrent tensor a_{ijkl}, given by

$$a_{ijkl} = \sum_{a,b,c,d} \delta_{abcd} P_{ia} P_{jb} P_{kc} P_{ld} \tag{1.22}$$

where the generalization of the Kronecker delta is defined as

$$\delta_{i_1 \ldots i_n} = \begin{cases} 1 & \text{if } i_1 = \ldots = i_n \\ 0 & \text{otherwise} \end{cases} \tag{1.23}$$

See ??. At the edges and corners, we have suitable 2 and 3 legged tensors, 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.

Figure 1.4: Hallo hier staat nog niks

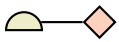

Figure 1.5: lalala nog niks

We can now redefine the row-to-row transfer matrix from Equation 1.12 as the tensor network expressed in Figure 1.5. For all l, it is still true that

$$Z_{N\times l} = \mathrm{Tr}\, T_N^l = \sum_{i=1}^{2^N} \lambda_i^l \tag{1.24}$$

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

$$T_{\text{new}} = P T_{\text{old}} P^{-1} \tag{1.25}$$

1.4 Transfer matrix renormalization group

More about connection between 1D quantum and 2D classical

Pictures

We will now focus on contracting the infinite tensor network of Figure 1.5. 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

$$\lim_{l\to\infty} T_N^l = \lim_{l\to\infty} (\lambda_0)_N^l \, |\lambda_0\rangle_N \langle\lambda_0|_N \sim |\lambda_0\rangle_N \langle\lambda_0|_N \tag{1.26}$$

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. (??))

$$\rho_N = |\Psi_0\rangle_N \langle\Psi_0|_N \tag{1.27}$$

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

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

$$A_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} = \begin{cases} \sum \prod_{\langle i,j,k,l\rangle} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l) & \text{if } \sigma_1 = \sigma_1' \\ 0 & \text{if } \sigma_1 \neq \sigma_1' \end{cases} \tag{1.28}$$

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

$$W(a, b, c, d) = W(b, a, d, c) = W(c, a, d, b) = W(d, c, b, a) \tag{1.29}$$

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

$$Z_{N\times N} = \mathrm{Tr} A^4 \tag{1.30}$$

In the thermodynamic limit, (1.30) is equal to (1.13).

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 [5].

2

Introduction to tensor networks

2.1 Tensors, or multidimensional arrays

Make clear that there is a difference between tensors that are defined with a metric.

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

$$v_i = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} \tag{2.1}$$

which has one index, and a matrix

$$M_{ij} = \begin{bmatrix} M_{11} & \dots & M_{1n} \\ \vdots & & \vdots \\ M_{m1} & \dots & M_{mn} \end{bmatrix} \tag{2.2}$$

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

$$T_{i_1 \dots i_N} \tag{2.3}$$

A tensor of rank zero is just a scalar.

[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.

2.2 Tensor contraction

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

$$\boldsymbol{a} \cdot \boldsymbol{b} = \sum_i a_i b_i \tag{2.4}$$

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

$$(M\boldsymbol{a})_i = \sum_j M_{ij} a_j \tag{2.5}$$

and matrix-matrix multiplication

$$(AB)_{ij} = \sum_k A_{ik} B_{kj}, \tag{2.6}$$

but a more elaborate tensor multiplication could look like

$$w_{abc} = \sum_{d,e,f} T_{abcdef} v_{def}\,. \tag{2.7}$$

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.

2.3 Tensor networks

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

$$M_{ab} = \sum_{i,j,k} A_{ai} B_{ij} C_{jk} D_{kb} \tag{2.8}$$

which corresponds to the matrix product $ABCD$.

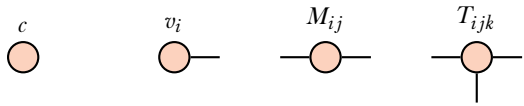

Figure 2.1: Open-ended lines, called legs, represent unsummed indices. A tensor with no open legs is a scalar.

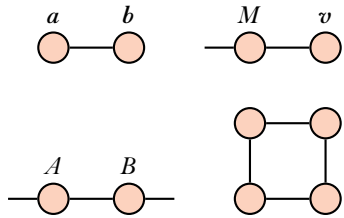

Figure 2.2: Connected legs represent contracted indices. The networks in the figure represent $\sum_i a_i b_i$ (dot product), $\sum_j M_{ij} a_j$ (matrix-vector product), $\sum_k A_{ik} B_{kj}$ (matrix-matrix product) and $\mathrm{Tr}\, ABCD$, respectively.

2.3.1 Graphical notation

It is highly convenient to introduce a graphical notation that is common in the tensor network community. It greatly simplifies expressions and makes certain properties manifest.

Each tensor is represented by a shape. Open-ended lines, called legs, represent unsummed indices. See Figure 2.1. Each contracted index is represented by a connected line. See Figure 2.2.

Many tensor equations, while burdensome when written out, are readily understood in this graphical way. As an example, consider the matrix trace in Figure 2.2, where its cyclic property is manifest.

2.3.2 Computational complexity of contraction

Computational complexity.

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