Master Engineering Physics

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Master desertatoin

Thesis Tensor networks

October 2020

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Academic supervisor: prof.

Contents

Todo list

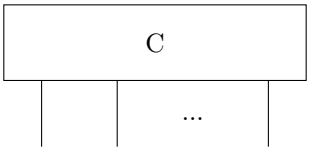


Figure 1: Caption

1 Introduction

blablabla

To deal with these strongly correlated systems, a class of methods called tensor networs were introced.

1.1 MPS

A general quantum state with n sites can be described in a given basis $|i\rangle$ as

$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \tag{1}$$

This requires an exponential number d^n of coefficients C where d is the dimensions of basis $|i\rangle$.

In order to make the problem tractable, the following form is proposed as wavefunction:

$$C^{i_1 i_2 \cdots i_n} = C^{1\,i_1}_{\alpha_1} C^{2\,i_2}_{\alpha_1 \alpha_2} \cdots C^{n\,i_n}_{\alpha_{n-1}} \tag{2}$$

Where summation over shared indices is implied. It is always possible to find such an representation by means of matrix decomposition. The summation over α_i are called virtual bond and their dimension is denoted by χ.

Explicit translational invariance is given by tensor $C^i_{\alpha\beta}$ that don't depend on the location. The chain is closed by setting $\alpha_n = \alpha_0$. We can now write this as a Trace over matrix products:

$$|\Psi\rangle = \mathrm{Tr}\left(C^{i_1} C^{i_2} \cdots C^{i_n}\right) |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \tag{3}$$

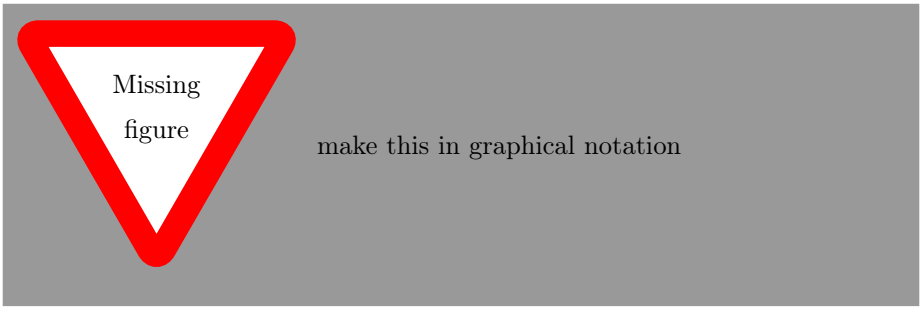
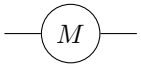
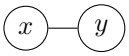


Table 1: Caption

conventional	Einstein	tensor notation
$\vec{x}$	x_α	
M	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	

1.2 graphical notation

Tensor networks can be written in a graphical notation. The legs f a tensor denote the number of external indices. The upper Connected legs are summed. Some examples are shown in table 1

1.3 MPO

In a similar fashion, a Matrix Product Operator (MPO) is of the following form:

$$\begin{aligned} \hat{O} = \sum Tr(A^{i_1 j_1} A^{i_2 j_2} \cdots A^{i_n j_n} M) \\ \times |i_1\rangle \langle j_1| \otimes |i_2\rangle \langle j_2| \otimes \cdots \otimes |i_n\rangle \langle j_n| \end{aligned} \tag{4}$$

The matrix M contains the boundary conditions of the operator.

1.4 PEPO

2 Statistical mechanics

In order to simulate quantum systems at finite temperatures, we need to construct statistical ensembles from the quantum states. An useful quantity is the density matrix ρ.

$$\begin{aligned} Z &= e^{-\beta E_n} \\ &= \sum_n \left\langle n \left| e^{-\beta \hat{H}} \right| n \right\rangle \\ &= \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \end{aligned} \tag{5}$$

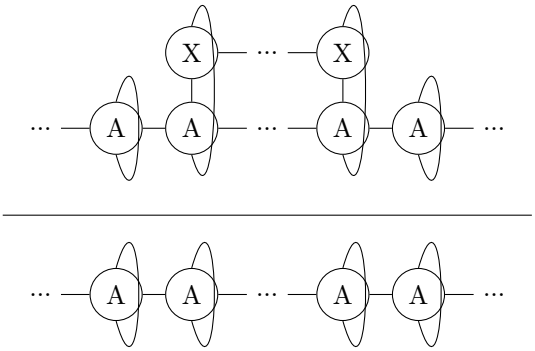
$$\rho = \sum_j \frac{e^{-\beta \hat{H}}}{Z} |\Psi_j\rangle \langle \Psi_j|) \tag{6}$$

$$
\begin{aligned}
Z &= \mathrm{Tr}(\rho) \\
\langle X \rangle &= \mathrm{Tr}\Big(\rho \hat{X}\Big)
\end{aligned}
\tag{7}
$$

2.1 Calculation with MPO in 1D

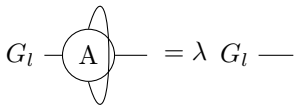
Suppose that the there is an MPO representation of $e^{-\beta \hat{H}}$ A and that the mpo represenation for X Y is localised over n sites, then the expactation value is given by:

$\langle X \rangle =$

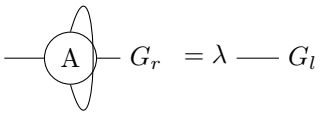


(8)

In the thermodynamic limit there are an infinity number of A to the left and the right. This can be simulated by taking the left and right fixed points of the traced MPO A corresponding to the largest eigenvector λ.

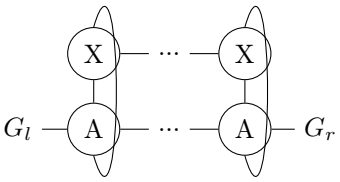


(9)



(10)

Equation eq. (8) can now be easily caclulated:



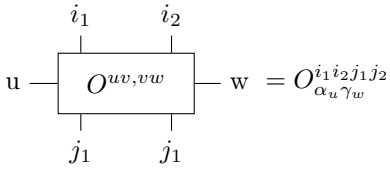
$$\langle X \rangle = \frac{}{\lambda^n \quad G_r \; G_r} \tag{11}$$

3 contruction MPO

3.1 Mpo manipulations

The manipulations of MPO's is done by manipulating the tensor into a matrix, performing some matrix calculations and casting it back into it's original form. This section gives some examples how these manipulations are done in practice:

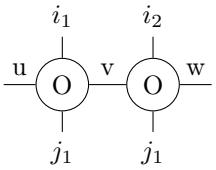
3.1.1 decomposition



$$= O^{i_1 i_2 j_1 j_2}_{\alpha_u \gamma_w}$$

$$\begin{aligned} &\cong O^{uw}_{(\alpha_u i_1 j_1)(\gamma_w i_2 j_2)} \\ &= O^{uv}_{(\alpha_u i_1 j_1)\beta_v} O^{vw}_{\beta_v (\gamma_w i_2 j_2)} \end{aligned} \tag{12}$$

$\cong$



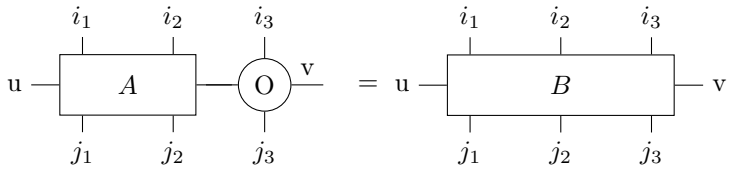
Step 2 reshapes and groups the indices to one index. The dimension of this index is the sum of the seperate dimensions. Step 3 decomposes the matrix into a product of 2 matrices. The exact nature of this decomposition is dicussed further. The last step transforms the indices back to separate legs.

For an exact representation, the bond dimension of virtual level v is:

$$\dim v = \min(\dim u, \dim v) + 2 \dim i \tag{13}$$

3.1.2 inverse

Suppose we want to find a MPO O for given tensors A and B such that the following holds:

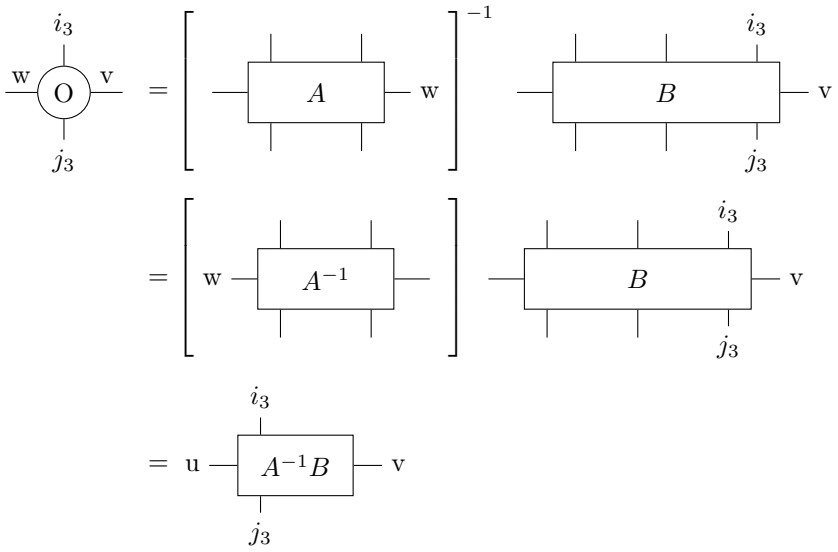


(14)

Again, the indices can be taken toghether in the following way: $\alpha = (ui_1i_2j_1j_2)$ and $\beta = (i_3j_3v)$:

$$A_{\alpha\gamma}O_{\gamma\beta} = B_{\alpha\beta} \tag{15}$$

This will be denoted by



(16)

For the first equation the unmarked legs on similar positions need to be connected to each other. The second line the mirrored positions are connected.

This can now be computed with linear algebra packages. Note that it is not necessary to calculate A^{-1} to obtain the solution.

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3.1.3 virtual levels and matrisation

explain

3.1.3.1 Matrisation From the construction with svd we can see that the dimension of virtual bond $\dim n = d^{2n}$ with d the dimension of $|i\rangle$. The virtual levels can be joined into a $\chi \times d \times d \times \chi$ dimensional tensor O. This tensor is given by a tridiagonal block matrix :

$$O^{ij}_{\alpha\beta} = \begin{bmatrix} O^{00,ij} & O^{01,ij} & & \\ O^{10,ij} & O^{11,ij} & O^{12,ij} & \\ & O^{21,ij} & O^{22,ij} & \ddots \\ & & \ddots & \ddots \end{bmatrix} \tag{17}$$

The boundary conditions (leftmost and rightmost virtual level are zero) correspond to vectors:

$$\begin{aligned} l &= \begin{bmatrix} 1 & 0 & \cdots \end{bmatrix} \\ r &= l^T \end{aligned} \tag{18}$$

The total dimension is the sum of dimensions of the virtual level. In this case the

berken exact en maak tabletje voor de verschillende types

3.2 Time evolution methods

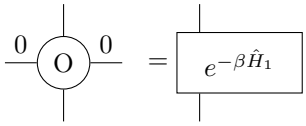
3.3 Cluster expansion

This thesis builds on the cluster expansions introduced in [1]. The idea is to create tensor network with a number of virtual levels. The representation is exact up to M connected sites, where M is the order. Different variations are possible.

A Hamiltonian of the folowing form is assumed

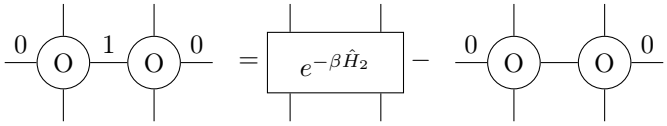
$$\hat{H}_n = \sum_{i=1}^{n-1} \hat{h}_{i,i+1} + \sum_{i=1}^{n} \hat{h'}_i \tag{19}$$

Virtual level zero is defined as follows:



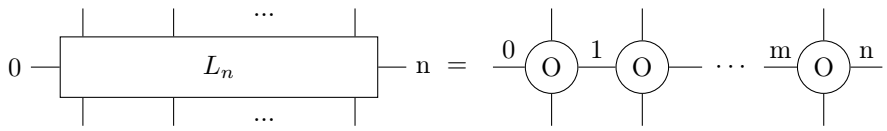
(20)

Similarly, the contraction of elements O_{01} and O_{10} are defined as follows:



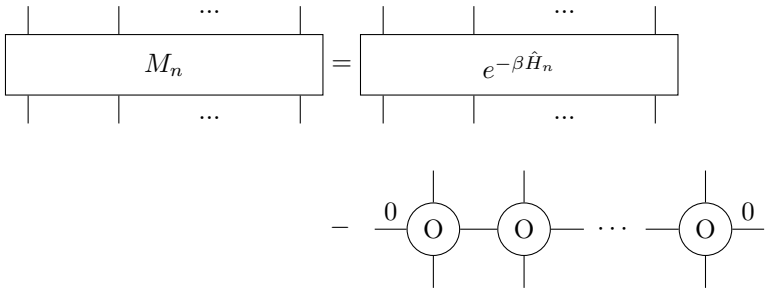
(21)

Some notation will be introduced that will be used later on. The rensor L_n is the contraction of n MPO's where the virtual index increases between each bond. R_n is similar but the virtual bond starts from n and decreases.



(22)

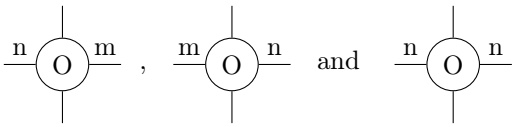
M_n is the difference between the exponentiated hamiltonian for n sites and the contraction of the MPO over all the currently assigned combinations of virtual levels.



(23)

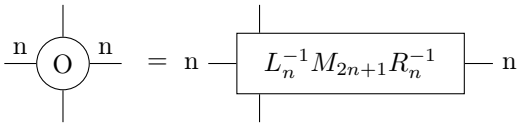
3.3.1 Type A

This type was originally proposed in [1]. The following types of blocks appear:



with $n \in \mathbb{N}_0$ and $m = n - 1$.

3.3.1.1 O^{nn} The O^{nn} block is defined by eq. (24)

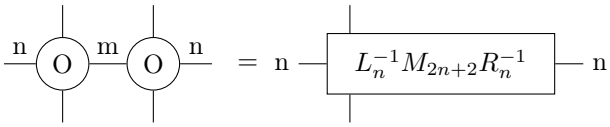


(24)

The residual error M is calculated for a chain of size $2n + 1$. The left and right inverses are applied to M to find the block O^{nn}

3.3.1.2 O^{mn} and O^{nm}

The contraction of O^{nm} and O^{mn} is defined by:



(25)

The individual elements O^{mn} and O^{nm} are obtained by doing an svd decoposition.

symmetric split S, invertibility lowest eiges, eigensplit, order cutoff

3.3.2 Truncation

Because the inverse is possibly ill conditioned, increasing the order does not always inprove accuracy. Therefore, criteria are needed to truncute the order at the optimal point.

3.3.2.1 O^{nn}

For this block 2 criteria need to be checked. First, the inverse needs to be well conditioned:

$$\begin{aligned} \mathcal{K} &= \frac{\sigma_{max}}{\sigma_{min}} \\ &< 10^5 \end{aligned} \tag{26}$$

It is also necesarry to check whether the added block really improves the error. Therefore, M_{2*n+2} is calculated with and without the new block. The singular values spectrum is calculated for the middle bond. The maximum error needs to decrease: $\sigma_{max,new} < \sigma_{max,new}$ and also the average error: $\sum \sigma_{i,new} < \sum \sigma_{i,new}$.

3.3.2.2 O^{mn} and O^{nm}

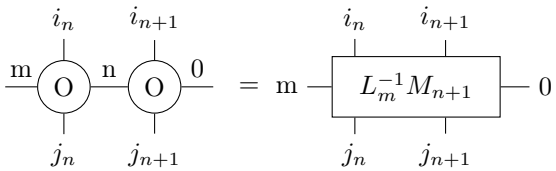
It is sufficient to check whether the maximum singular value and the average singular values have decreased.

3.3.3 discussion

blabla

3.3.4 Type B

Type B only contains blocks of the following form; O^{mn} and O^{n0}

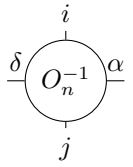


$$\begin{aligned} &\cong X_{(\alpha_m i_n j_n)(i_{n+1} j_{n+1})} \\ &= U^n \Sigma V^\dagger \end{aligned} \tag{27}$$

The following split is made: $O^{mn} \cong U^n$ and $O^{n0} \cong \Sigma V^\dagger$. In this way the inverse exists and doesn't need any calculation: $O^{mn} = U^\dagger$. Take has to be taken with the indices to apply the inverse.

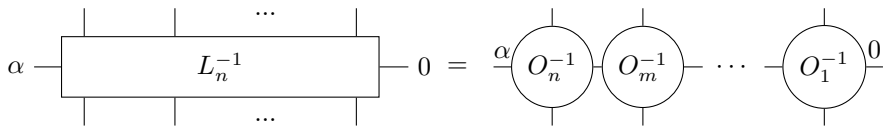
$$\begin{aligned} U^n_{(\alpha ij)\beta} A_{\beta\gamma} &= B_{\alpha ij\gamma} \\ A_{\delta\gamma} &= U^{n\dagger}_{\delta(\alpha ij)} B_{\alpha ij\gamma} \end{aligned} \tag{28}$$

If we now define the MPO O_n^{-1} equal to $U^{n\dagger}$ with the second index split and permuted:



$$\cong U^{n\dagger}_{\delta ij\alpha} \tag{29}$$

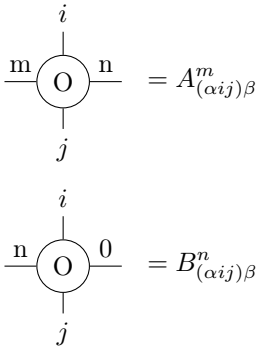
With the notation from eq. (16) we have:



(30)

The inverse can be applied sequentially.

3.3.4.1 dimension From the construction the bond dimension grows from the left to the right. Again $\dim n = d^{2n}$. However this can be reduced if we can solve the following equations simultaneously:



(31)

Then the MPO doesn't change if there are matrices A'^n, A'^{n+1} and B'^n such that

$$\begin{aligned} S &= A^m A^n = A'^m A'^n \\ T &= A^m B^n = A'^m B'^n \end{aligned} \tag{32}$$

Such matrices with optimal bond dimension can be found with generalised SVD. Generalised SVD decomposes 2 matrices as follows

$$\begin{aligned} S^\dagger &= (U\Sigma_1)Q^\dagger \\ T^\dagger &= (V\Sigma_2)Q^\dagger \end{aligned} \tag{33}$$

As expected, the bond dimension is the $\dim n' = \min(d^2 \dim m, \dim(n+1)d^2)$.

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3.3.4.2 discussion

3.3.5 Type C

primed virtual levels

3.3.6 Type D

4 Benchmark 1D cluster expansion

4.1 Ising model

4.1.1 Classical Ising

The classical ising model is given by the following hamiltonian

$$H = \sum_{<ij>} \sigma_i \sigma_j + \sum_i \sigma_i \tag{34}$$

4.1.2 transversel

The quantum ising chain is given by the following hamiltonian:

$$H = \sum_i S \tag{35}$$

4.2 Heisenberg

test 2

4.3 Random

References

[1] B. Vanhecke, M. Damme, L. Vanderstraeten, F. Verstraete, Symmetric cluster expansions with tensor networks (12 2019).