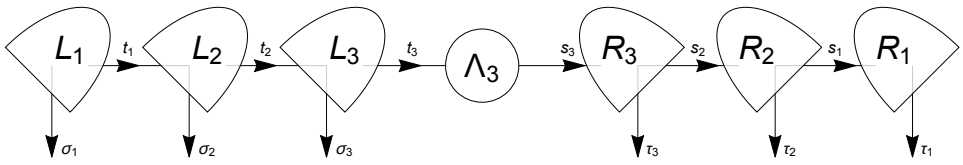
Chapter 5

Optimizing Matrix Product States – iDMRG

A. Infinite DMRG

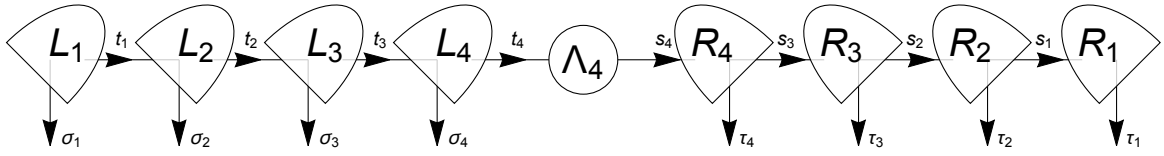
Our first algorithm will be the "Infinite Density Matrix Renormalization Group" or iDMRG. If I understand my history correctly, this was the first "Density Matrix Renormalization Group." It is a beautiful algorithm. It is easy to code though, and introduces all of the structure that we need..

It is an iterative technique. Imagine that we have a wavefunction which is a good estimate to the ground state of the six-site problem

$|\psi_6\rangle =$ 

. (5.1)

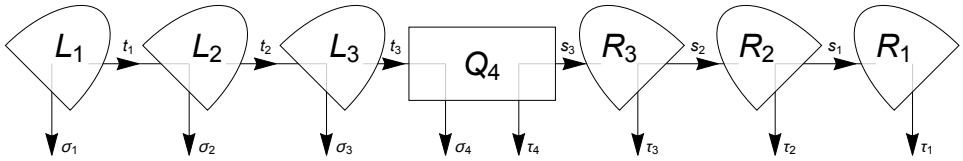
Here we have indexed the left three spins as $\sigma_1, \sigma_2, \sigma_3$, and the right three as τ_3, τ_2, τ_1. Our goal is to find the L_4, R_4, Λ_4 which give us the best approximation to the ground state on 8-sites

$|\psi_8\rangle =$ 

, (5.2)

with some constraint on the bond dimension χ. The idea is that we keep repeating this procedure, we will find that it converges to a fixed point $L_j, R_j, \Lambda_j = L_{j-1}, R_{j-1}, \Lambda_{j-1} = L, R, \Lambda$. At that point we have constructed the optimal infinite matrix product state with fixed χ.

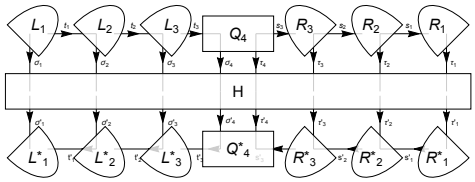
We will first solve a slightly bigger problem, optimizing a wavefunction of the form

$|\tilde{\psi}_8\rangle =$ 

. (5.3)

Once we have found Q, we use a singular value decomposition to produce L, R, and Λ.

Our optimization criterion will be energy – that is we want to find Q which minimizes

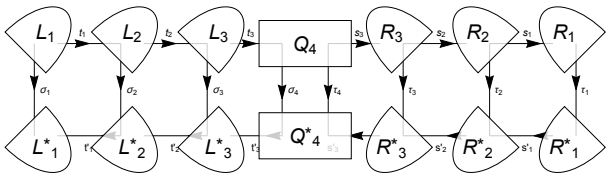
$\langle H \rangle =$ 

(5.4)

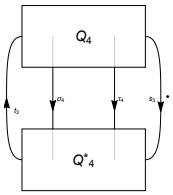
subject to the constraint

$$\langle \psi | \psi \rangle \quad = \quad 1. \tag{5.5}$$

The normalization can be written

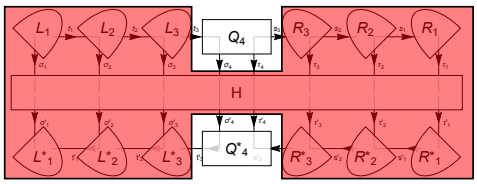
$\langle \psi | \psi \rangle \quad =$ 

(5.6)

$=$ 

. (5.7)

We group together the tensors in red to make a matrix H_4, and tie the indices $s_3, t_3, \sigma_4, \tau_4$ together to make one index

$Q^\dagger H_4 Q \quad =$ 

. (5.8)

Here Q is interpreted as a vector of length$\chi \times \chi \times d \times d$, where χ is the number of values taken on by each of t and s, while d is the number of values taken on by each of σ and τ. Clearly H_4 is a $\chi^2 d^2 \times \chi^2 d^2$ Hermitian matrix. In this notation, the normalization condition is

$$Q^\dagger Q = 1. \tag{5.9}$$

You should be familiar with the idea that if you minimize $Q^\dagger H_4 Q$ with the constraint $Q^\dagger Q = 1$, that is equivalent to solving the eigenvalue problems

$$H_4 Q = EQ, \tag{5.10}$$

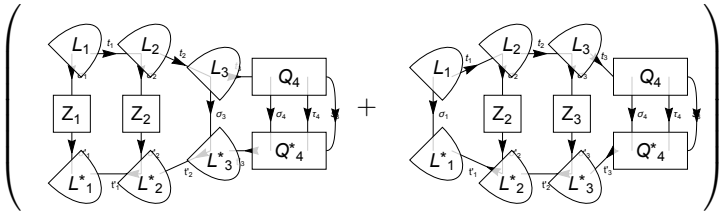
where the eigenvalue E is the energy.

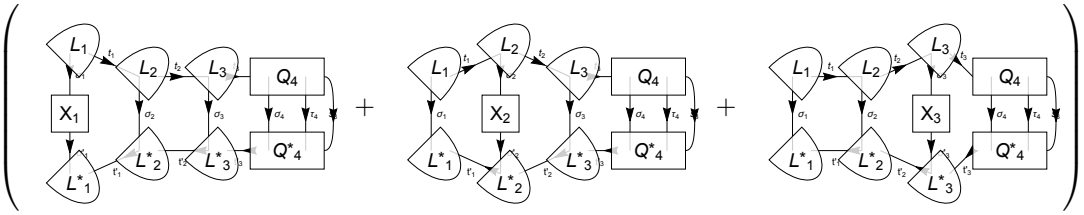
The only other thing we need to think about is calculating H_4. Lets specialize to the case of the transverse field Ising Model

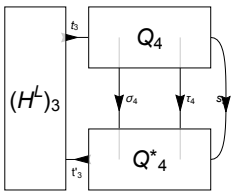
$$H = -J \sum_j Z_j Z_{j+1} - h \sum_j X_j, \tag{5.11}$$

where $Z_j = \sigma_j^z$, and $X_j = \sigma_x^j$ are Pauli matrices.

In the present case (where we are thinking about 8 spins) there are 15 terms, which are naturally grouped into five categories, $H = H^{LL} + H^{LC} + H^{CC} + H^{CR} + H^{RR}$. If we had longer range couplings, we may also have H_{LR} terms. The expectation values of the left terms are

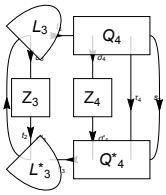
$\langle H^{LL} \rangle$ = $-J$  (5.12)

$-h$ 

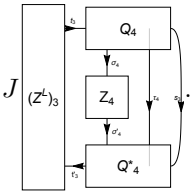
=  (5.13)

which defines the matrix H^L. The terms joining the left and central region are

$$\langle H^{LC} \rangle = -J \tag{5.14}$$

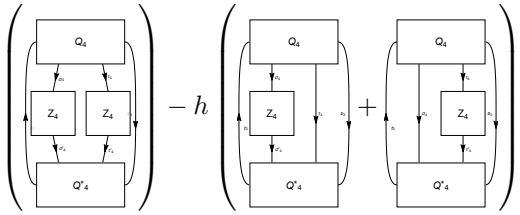


$$= -J \tag{5.15}$$



The terms just involving the center are

$$\langle H^{CC} \rangle = -J \tag{5.16}$$



There is no need to draw the terms for the right, since they are just mirror images of the left.

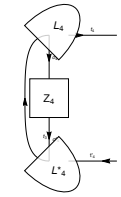
Putting everything together, we start with the following matrices:

- H_3^L**:** A $\chi \times \chi$ matrix which describes the Hamiltonian on the left, written in the Schmidt basis.
- Z_3^L**:** A $\chi \times \chi$ matrix which describes the Z operator acting on the third site, written in the Schmidt basis.
- H_3^R**:** A $\chi \times \chi$ matrix which describes the Hamiltonian on the right, written in the Schmidt basis – note that by symmetry this can typically be taken to be equal to H_3^L
- Z_3^R**:** A $\chi \times \chi$ matrix which describes the Z operator acting on the third site from the right, written in the Schmidt basis – note that by symmetry this can typically be taken to be equal to H_3^L.

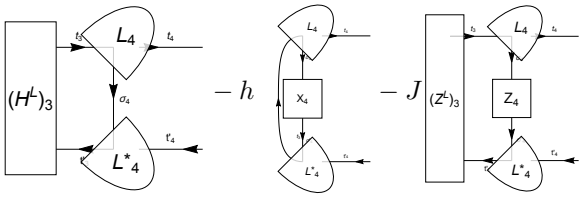
Suppose we have symmetry, so we only need the first two. We use these to construct H_4. We find the lowest

energy state Q_4 and energy E_4. We then do a SVD to construct L_4 and Λ. We then construct

$$Z_4^L = \tag{5.17}$$



$$H_4^L = \tag{5.18}$$



$$- \frac{E_4}{2}\mathbf{1}.$$

Where the last term is proportional to the identity matrix. We subtract off half the energy to keep the operator bounded (it is only half, because the other half is absorbed by the right). Effectively this means that when we calculate the next energy, we are just finding out how much energy is added by the two new sites. After j iterations, our best estimate of the energy per site is $E_j/2$.

We now have everything we need for the next iteration. Note: We don't even need to store the L matrices (though we can store the latest L and use it to seed out eigenvalue solver – one of the homeworks describes how to use it).

B. Starting Out

One good question is what to use for the first iteration. It turns out the best idea is to use a starting H_L and Z_L which breaks the up-down symmetry. If you don't you will end up with a Schrodinger cat state – which requires twice the bond dimension, and is poorly behaved. A good choice is to start with bond dimension 1, and use

$$H_L = 0 \tag{5.19}$$

$$Z_L = 1. \tag{5.20}$$

Spend the rest of class beginning to implementing this algorithm in Mathematica, using the template notebook. Finishing it will be part of your homework. I'll walk around and help.

C. Homework 4

Problem 22. Finish writing the IDMRG Code that we started in class, and do the exercises at the end of the notebook.