

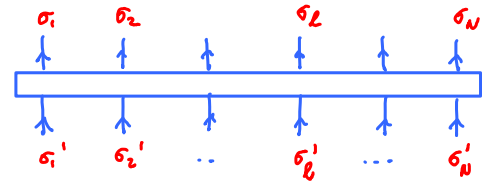
[credit for course materials: Prof. Jan von Delft]

Matrix product operators; DMRG

Matrix product operators

[Schollwöck2011, Sec 5]

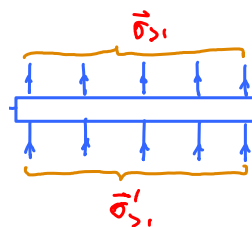
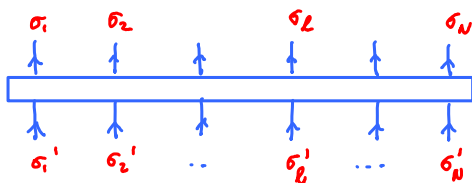
Consider an operator acting on N-site chain:



It can always be written as a

'matrix product operator' (MPO)

using a sequence of QR decompositions:



In general, this produces MPO
with growing bond dimensions.

But for short-range Hamiltonians, bond dimension is typically small.

1. Applying MPO to MPS yields MPS

with composite indices,

of increased dimension:

In practice, application of MPO is usually followed by SVD+truncation to bring bond dimension back down:

Addition of MPOs:

Let

= MPO in enlarged space

Multiplication of MPOs

with composite indices, of increased dimension

2. MPO representation of Heisenberg Hamiltonian

is shorthand for

Contains sum of one and two-site operators. How can we write it as an MPO?

Solution: introduce operator-valued matrices such that product reproduces above form!

Each \hat{S}^{α} acts only on site i ; their tensor product gives the full MPO.

Viewed from a bond, the string of operators in each term of \hat{S}^{α} can be in one of five states.



- state 1: only \hat{S}^z to the right
- state 2: only \hat{S}^+ just to the right
- state 3: one \hat{S}^+ just to the right
- state 4: one \hat{S}^- just to the right
- state 5: one \hat{S}^z or completed interaction somewhere to the right

Build matrix with element

implements transition from 'state'

to

$$\hat{W}_{[l]} = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} \underline{1} & 0 & & & \\ \hat{S}^+ & 0 & & & \\ \hat{S}^- & 0 & & & \\ \hat{S}^z & 0 & 0 & 0 & 0 \\ -h\hat{S}^z & \frac{J}{2}\hat{S}^- & \frac{J}{2}\hat{S}^+ & J^z\hat{S}^z & \hat{1} \end{bmatrix} \end{matrix}$$

On site N:

$$\hat{W}_{[N]} = \begin{matrix} & \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} \hat{1} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -h\hat{S}^z \end{bmatrix} \end{matrix}$$

and also column 1 of $\hat{W}_{[l]}$

One site 1 (= row 1 of $\hat{W}_{[l]}$):

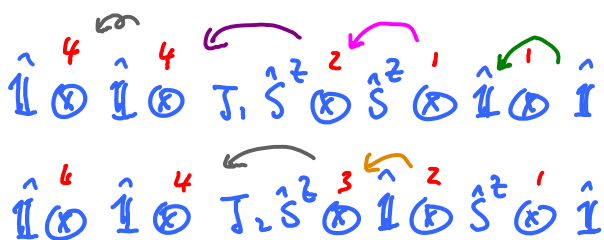
$$\hat{W}^{[1]} = [-h\hat{S}^z, \frac{J}{2}\hat{S}^-, \frac{J}{2}\hat{S}^+, J^z\hat{S}^z, \hat{1}]$$

Check: multiplying out a product of such 's yields desired result:

$$\begin{aligned}
 \hat{w}_{[1]} \hat{w}_{[2]} \hat{w}_{[3]} \hat{w}_{[4]} &= \hat{w}_{[1]} \hat{w}_{[2]} \begin{pmatrix} \hat{1} & 0 \\ \hat{s}^+ & 0 \\ \hat{s}^- & 0 \\ \hat{s}^z & 0 \\ -\mathcal{L}\hat{s}^z & \frac{1}{2}\hat{s}^- & \frac{1}{2}\hat{s}^+ & J^z\hat{s}^z & \hat{1} \end{pmatrix} \begin{pmatrix} \hat{1} \\ \hat{s}^+ \\ \hat{s}^- \\ \hat{s}^z \\ -\mathcal{L}\hat{s}^z \end{pmatrix} \\
 &= \hat{w}_{[1]} \begin{pmatrix} \hat{1} & 0 \\ \hat{s}^+ & 0 \\ \hat{s}^- & 0 \\ \hat{s}^z & 0 \\ -\mathcal{L}\hat{s}^z & \frac{1}{2}\hat{s}^- & \frac{1}{2}\hat{s}^+ & J^z\hat{s}^z & \hat{1} \end{pmatrix} \begin{pmatrix} \hat{1} \otimes \hat{1} \\ \hat{s}^+ \otimes \hat{1} \\ \hat{s}^- \otimes \hat{1} \\ \hat{s}^z \otimes \hat{1} \\ (-\mathcal{L}\hat{s}^z \otimes \hat{1} + \frac{1}{2}\hat{s}^- \otimes \hat{s}^+ + \frac{1}{2}\hat{s}^+ \otimes \hat{s}^- + J^z\hat{s}^z \otimes \hat{s}^z + \hat{1} \otimes (-\mathcal{L}\hat{s}^z)) \end{pmatrix} \\
 &= [-\mathcal{L}\hat{s}^z, \frac{1}{2}\hat{s}^-, \frac{1}{2}\hat{s}^+, J^z\hat{s}^z, 1] \begin{pmatrix} \hat{1} \otimes \hat{1} \otimes \hat{1} \\ \hat{s}^+ \otimes \hat{1} \otimes \hat{1} \\ \hat{s}^- \otimes \hat{1} \otimes \hat{1} \\ \hat{s}^z \otimes \hat{1} \otimes \hat{1} \\ (-\mathcal{L}\hat{s}^z \otimes \hat{1} \otimes \hat{1} + \frac{1}{2}\hat{s}^- \otimes \hat{s}^+ \otimes \hat{1} + \frac{1}{2}\hat{s}^+ \otimes \hat{s}^- \otimes \hat{1} + J^z\hat{s}^z \otimes \hat{s}^z \otimes \hat{1} \\ + \hat{1} \otimes (-\mathcal{L}\hat{s}^z) \otimes \hat{1} + \hat{1} \otimes \frac{1}{2}\hat{s}^- \otimes \hat{s}^+ + \hat{1} \otimes \frac{1}{2}\hat{s}^+ \otimes \hat{s}^- + \hat{1} \otimes J^z\hat{s}^z \otimes \hat{s}^z \\ + \hat{1} \otimes \hat{1} \otimes (-\mathcal{L}\hat{s}^z)) \end{pmatrix} \\
 &= -\mathcal{L}\hat{s}^z \otimes \hat{1} \otimes \hat{1} \otimes \hat{1} + \frac{1}{2}\hat{s}^- \otimes \hat{s}^+ \otimes \hat{1} \otimes \hat{1} + \frac{1}{2}\hat{s}^+ \otimes \hat{s}^- \otimes \hat{1} \otimes \hat{1} + J^z\hat{s}^z \otimes \hat{s}^z \otimes \hat{1} \otimes \hat{1} \\
 &\quad + \hat{1} \otimes (-\mathcal{L}\hat{s}^z) \otimes \hat{1} \otimes \hat{1} + \hat{1} \otimes \frac{1}{2}\hat{s}^- \otimes \hat{s}^+ \otimes \hat{1} + \hat{1} \otimes \frac{1}{2}\hat{s}^+ \otimes \hat{s}^- \otimes \hat{1} + \hat{1} \otimes J^z\hat{s}^z \otimes \hat{s}^z \otimes \hat{1} \\
 &\quad + \hat{1} \otimes \hat{1} \otimes (-\mathcal{L}\hat{s}^z) \otimes \hat{1} + \hat{1} \otimes \hat{1} \otimes \frac{1}{2}\hat{s}^- \otimes \hat{s}^+ + \hat{1} \otimes \hat{1} \otimes \frac{1}{2}\hat{s}^+ \otimes \hat{s}^- + \hat{1} \otimes \hat{1} \otimes J^z\hat{s}^z \otimes \hat{s}^z \\
 &\quad + \hat{1} \otimes \hat{1} \otimes \hat{1} \otimes (-\mathcal{L}\hat{s}^z)
 \end{aligned}$$

= full Hamiltonian for 4 sites! ✓

Longer-ranged interactions



- state 1: only to the right
- state 2: only just to the right
- state 3: one just to the right
- state 4: completed interaction somewhere to the right

$$\hat{W}_{[2]} = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{pmatrix} \hat{1} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \hat{1} & 0 & 0 \\ 0 & J_1 \hat{S}^z & J_2 \hat{S}^z & \hat{1} \end{pmatrix} \end{matrix}$$

$$\hat{W}_{[N]} = \begin{pmatrix} \hat{1} \\ \hat{S}^z \\ 0 \\ 0 \end{pmatrix} = \text{column } 1 \text{ of } \hat{W}_{[2]}$$

$$\hat{W}_{[1]} = (0, J_1 \hat{S}^z, J_2 \hat{S}^z, \hat{1}) = \text{row } 4 \text{ of } \hat{W}_{[2]}$$

Check:

$$\hat{W}^{(1)} \hat{W}^{(2)} \hat{W}^{(3)} = \hat{W}^{(1)} \begin{pmatrix} \hat{1} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \hat{1} & 0 & 0 \\ 0 & J_1 \hat{S}^z & J_2 \hat{S}^z & \hat{1} \end{pmatrix} \begin{pmatrix} \hat{1} \\ \hat{S}^z \\ 0 \\ 0 \end{pmatrix}$$

$$= (0, J_1 \hat{S}^z, J_2 \hat{S}^z, \hat{1}) \begin{pmatrix} \hat{1} \otimes \hat{1} \\ \hat{S}_2^z \otimes \hat{1} \\ \hat{1} \otimes \hat{S}^z \\ 0 + J_1 \hat{S}_2^z \otimes \hat{S}^z + 0 + 0 \end{pmatrix}$$

$$= J_1 \hat{S}_2^z \otimes \hat{S}^z \otimes \hat{1} + J_2 \hat{S}_2^z \otimes \hat{1} \otimes \hat{S}^z + \hat{1} \otimes J_1 \hat{S}_2^z \otimes \hat{S}_2^z \quad \checkmark$$

3. Applying MPO to mixed-canonical state

[Schollwock2011, Sec 6.2]

How does an MPO act on an MPS in mixed-canonical representation wrt site ?

Consider

Here form a basis for the mixed-canonical representation. Express operator

in this basis:

then

L can be computed iteratively, for

(Similarly for R, for)

For efficient computation, perform sums in this order:

1. Sum over for fixed at cost
2. Sum over for fixed at cost
3. Sum over for fixed at cost

The application of MPO to MPS is then represented as:

DMRG I: Ground state search

- The density matrix renormalization group (DMRG) was invented by Steve White (student of Ken Wilson) to solve general quantum chain models. [White1992, 1993]
- First realization of connection between MPS and DMRG in limit : Ostlund & Rommer [Ostlund 1995]
- Realization that finite-size DMRG leads to MPS: Dukelski, Martin-Delgado, Nishino, Sierra [Dukelski1998]
- Modern formulation: Vidal [Vidal2003, 2004], Cirac and Verstraete [Verstraete2004]
- Time evolution: Daley, Kollath, Schollwock, Vidal [Daley2004], White, Feiguin [White2004]

1. Iterative ground state search

View space of all MPS of given bond dimension, χ , as variational space.

Minimize $\langle H \rangle$ in this space, subject to constraint of unit normalization,

Hence extremize:

Graphical representation, assuming mixed-canonical form wrt to site i :

Do this one tensor at a time:

In index notation:

This is an eigenvalue equation for λ can be solved with standard linear algebra tools such as a Lanczos algorithm.

Note: if \mathbf{A} is not represented in mixed-canonical form, one obtains a generalized eigenvalue equation of the form $\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x}$ with \mathbf{B} defined above.

Use that 'eigenvector' yielding lowest eigenvalue (=current estimate of ground state energy) to 'update' MPS, then move to next site, switch to mixed-canonical form on site ,
optimize , etc.

'Sweep' back and forth until convergence of ground state energy has been achieved.

This works remarkably well for 1D chains with short-ranged interactions.

2. Lanczos method

[Lanczos1950, Ojalvo1970, Paige1972, Koch2011]

- Fast way of finding extremal eigenvalues of a Hermitian $N \times N$ matrix, .
- Prerequisite: an algorithm for computing , for any vector .

We seek the extremal value of

Denote extremal value by

The direction of steepest ascent of the functional evaluated at is given by

‘functional gradient’:

Moving in opposite direction will thus lower the energy:

To find optimal value for α , minimize $\langle H \rangle$ wrt to 'variational parameter' α ,
in the space

Construct a normalized basis for this space (for a random initial state ψ):

First basis vector:

Second basis vector:

Now find a matrix representation of H in this space. Define:

then

Hence in the space \mathcal{S} , the Hamiltonian has the matrix representation:

The ground state of ψ , say ψ_0 , yields the optimal choice for ψ .

Now we could iterate: use ψ_0 as starting point for another optimization step.

Convergence is rapid. Monitor quality of result by computing the residual energy variance,

and stop when it drops below some threshold.

Krylov space

After n steps, starting from ψ_0 , the resulting vector will live in

= 'Krylov space of ψ_0 over \mathcal{H} ' (dimension n).

Instead of repeatedly minimizing in 2x2 subspaces, we could first construct \mathcal{K}_n , then compute its ground state. (This way is faster, since it amounts to using simultaneous variational parameters instead of n separate ones). To do this, iteratively construct a 'Krylov basis' for \mathcal{K}_n :

Krylov basis

As before:

Third vector:

where

Note:

Fourth vector:

Thus we obtain a two-term iteration scheme: we only need to store 3 vectors at a time!

n th step:

with

[If it happens that $\|v_n\| = 0$, pick an arbitrary v_n orthonormal to all v_1, \dots, v_{n-1}].

Throughout we have

since

Hence, rearranging:

So in \mathcal{K}_M , H has tridiagonal form:

Ground state of H_M satisfies the eigenvalue equation

Thus

$\{ \psi_k \}_{k=1}^M$ are the best approximations, within the Krylov space \mathcal{K}_M , of the true ground state energy and ground state.

Note: can be constructed 'on the fly', one term at a time, by restarting Lanczos iteration from .

The Lanczos scheme converges exponentially fast, with a rate constant \sim [gap to first excited state] .

Summary

1. Start with arbitrary
2. First iteration step

3. General iteration step for :

and repeat 3 until convergence.

There are other ways of organizing this iteration loop, but this one is most numerically stable [Paige1972]

3. DMRG for excited states

Suppose we have an MPS representation for ground state,

found by DMRG. Excited states can be constructed by repeating a DMRG sweep in space orthogonal to .

Extremize:

Lagrange multipliers enforce

Extremization wrt yields:

Generic structure of this equation, in mixed-canonical representation of site

Index-free notation:

Define projector onto subspace orthogonal to \mathbf{v} :

[with indices:

Project eigenvalue equation into this subspace:

This is simply an eigenvalue problem, for ψ , in subspace orthogonal to ψ_0 . It can be solved using straightforward generalization of Lanczos scheme, using Krylov subspace orthogonal to ψ_0 .

Given an arbitrary initial state ψ , project it onto orthogonal subspace, and construct new Krylov vectors using

Why not simply use excited states in ψ_0 ? Because numerical noise can cause the to be not exactly orthogonal, hence for $\langle \psi_0 | \psi \rangle$ rather than 0.

This leads to spurious multiple copies of eigenstates ('ghost states'). For the ground state, the variational principle ensures that the loss of orthogonality does not become a severe problem. But for excited states, it does. To prevent this, explicit reorthogonalization is needed at every step, using ψ_0 , as above.

Block-Lanczos for excited states

Standard Lanczos: represent action of H as

Block-Lanczos: start with set of orthogonal vectors,

, and represent action of H as

etc. Then the lowest M eigenstate of block-tridiagonal matrix

gives the Lanczos approximation for lowest M eigenstates of H

4. Two-site update

If one encodes symmetries, then 'one-site update' as discussed above can get stuck: if one starts in the wrong symmetry sector, one stays there, because one-site update offers no way of enlarging the Hilbert space during the variational search to explore other symmetry sectors. Cure: 'two-site' update, which variationally optimizes two A-tensors at a time.

Represent MPS in mixed-canonical two-site basis:

Then extremize simultaneously wrt

Compact notation: \tilde{H} with composite index
and

Use Lanczos to find lowest eigenvalue of variational equation, reshape updated \tilde{H} :
updated

Key point: \tilde{H} has dimensions 2^L , hence explores a larger state space than
previously, in general also including different symmetry sectors!

Truncate down to $2M$ and reshape;

This concludes optimization of \tilde{H} . Now move one site to right and repeat. Sweep
back and forth until convergence of full chain.