Matrix Product Operators

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Outline

Ian McCulloch

- Originally from Tasmania, Australia

- PhD at Australian National University, Canberra (2002)
- Europe (Netherlands, Gemany) until 2007
- University of Queensland, 2007 - 2023
- Now at National Tsing Hua University, Hsinchu
- NTHU Physics Department, room 715
- Email `mailto:ian@mx.nthu.edu.tw` (or `ian@phys.nthu.edu.tw` ??)
- MPS codes – see `https://mptoolkit.qusim.net`

DMRG Introduction

$$|\psi\rangle = \psi_{ij}\, |i\rangle_L |j\rangle_R$$

$$\rho = \psi\psi^\dagger$$

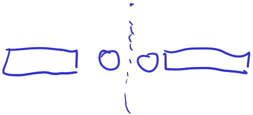
$$\rho_{ii'} = \sum_j \psi_{ij}\, \psi^*_{i'j}$$

$$\vec{S}_i \cdot \vec{S}_j = S^z_i S^z_j + \frac{1}{2}\left(S^+_i S^-_j + S^-_i S^+_j\right)$$

spin $s = \frac{1}{2}$

See code at `https://mptoolkit.qusim.net/Tutorials/SimpleDMRG`

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + h \sum_i S^z_i$$



$$\hat{H}' = \hat{H} \otimes I + \frac{1}{2}\left(\hat{S}^+ \otimes S^- + \hat{S}^z \otimes S^z + \hat{S}^- \otimes S^+\right)$$

Matrix Product States & Operators

If we look at the structure of the DMRG code, it can be written in a more expressive way using Matrix Product States and Matrix Product Operators

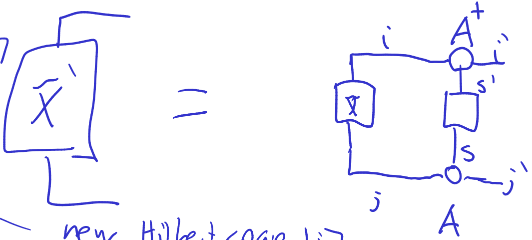
Merge Kronecker product and truncation

$$\tilde{X}' = T^\dagger (X \otimes \text{site})\, T$$

new site $|s\rangle$

$A^{s}_{ij'}$

old Hilbert space $|i\rangle$



new Hilbert space $|j\rangle$

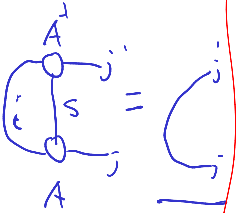
$$\tilde{X}'_{i'j'} = \sum_{ij} \sum_{s's} A^{s'\dagger}_{ii'} X_{ij} A^{s}_{jj'} \langle s' | \text{site} | s \rangle$$

assume $|i\rangle$ is orthogonal. (and normalized)

Want new basis $|j\rangle$ is also orthonormal.

$$\langle j'|j\rangle = \delta_{j'j}$$

$$\sum_{i,s} A^{s\dagger}_{ij'} A^{s}_{ij} = \delta_{j'j}$$



MPS – independent of DMRG construction

Method 1: quantize a classical state

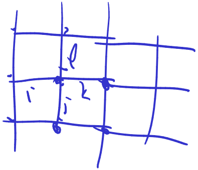
Start from a *classical* (product) state

A^{s}_{ijkl}

$$|\psi\rangle = |s^1\rangle\ |s^2\rangle\ |s^3\rangle\ |s^4\rangle\ \cdots$$

Each $|s^i\rangle$ is a classical vector, with real (or c-number) coefficients in some basis

$$|s^i\rangle = a_i^x|x\rangle + a_i^y|y\rangle + a_i^z|z\rangle$$



Turn our (commuting) numeric coefficients into a matrix

$$|s^i\rangle_{jk} = A_{jk}^x|x\rangle + A_{jk}^y|y\rangle + A_{jk}^z|z\rangle$$

We can recover an amplitude at the end by taking the trace, or arranging that the boundary matrices are $1 \times D$ and $D \times 1$.

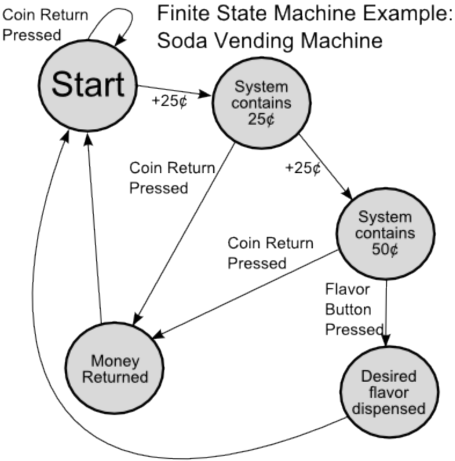
$$|\psi\rangle = \mathrm{Tr}\sum_{s_i} A^{s_1}A^{s_2}A^{s_3}A^{s_4}\cdots|s^1\rangle\ |s^2\rangle\ |s^3\rangle\ |s^4\rangle\cdots$$

Method 2: quantum finite-state machines

What is a Matrix Product State?

- Another way to visualizing them (from Greg Crosswhite)

A *finite-state machine* is a model of a system that can transition between a finite number of states.

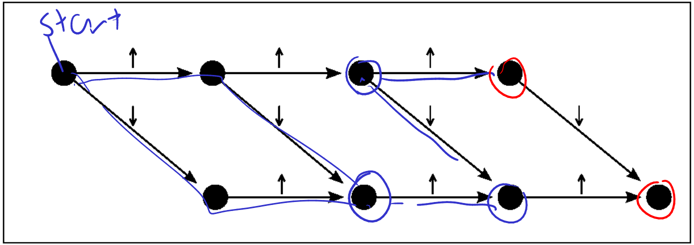


A classical finite-state machine is always in one discrete state.

$|\uparrow\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\uparrow\rangle$

In a *quantum* finite-state machine, we choose every possible transition with some probability amplitude

$|\uparrow\uparrow\uparrow\uparrow\rangle$



$|\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\uparrow\rangle$

(from Crosswhite and Bacon, Phys. Rev. A 78, 012356 (2008))

$|\uparrow\rangle \to |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle$

$|\downarrow\rangle \to |\downarrow\uparrow\rangle$

$$|\psi\rangle = \begin{cases} |\uparrow\rangle \\ |\downarrow\rangle \end{cases}$$

$|\uparrow\uparrow\rangle$

$|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle$

$\boxed{\text{W-state}}$

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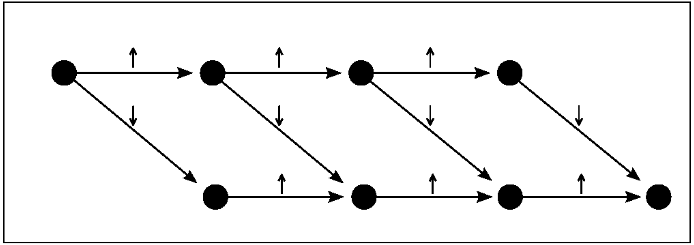

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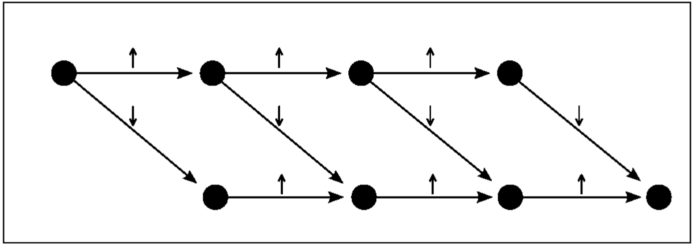

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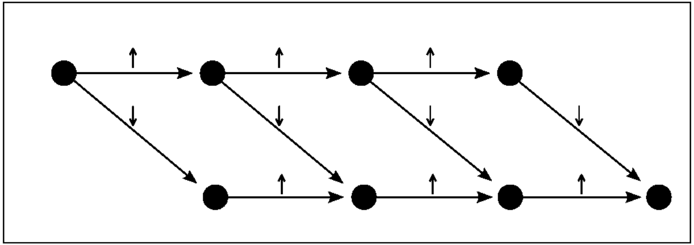


(from Crosswhite and Bacon, Phys. Rev. A 78, 012356 (2008))

$$|\psi\rangle = |{\downarrow\uparrow\uparrow\uparrow}\rangle + |{\uparrow\downarrow\uparrow\uparrow}\rangle + |{\uparrow\uparrow\downarrow\uparrow}\rangle + |{\uparrow\uparrow\uparrow\downarrow}\rangle$$

Matrix Product States

This quantum finite-state machine has a transition matrix associated with it

$$A^{|\downarrow\rangle} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

- W-state

$$|\psi\rangle = \frac{1}{\sqrt{N}}\left(|{\downarrow}{\uparrow}{\uparrow}{\uparrow}\ldots\rangle + |{\uparrow}{\downarrow}{\uparrow}{\uparrow}\ldots\rangle + |{\uparrow}{\uparrow}{\downarrow}{\uparrow}\ldots\rangle + \ldots\right)$$

$$A^{|\uparrow\rangle} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$A^s_{ij}$$

$$A = \begin{pmatrix} |\uparrow\rangle & |\downarrow\rangle \\ 0 & |\uparrow\rangle \end{pmatrix}$$

Practically all prototype wavefunctions studied in quantum information have a low-dimensional MPS representation

- GHZ state – long-range entangled, $S = \ln 2$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|{\uparrow}{\uparrow}{\uparrow}\ldots\rangle + |{\downarrow}{\downarrow}{\downarrow}\ldots\rangle\right)$$

$$A = \begin{pmatrix} |\uparrow\rangle & 0 \\ 0 & |\downarrow\rangle \end{pmatrix}$$

- AKLT state

$$A = \begin{pmatrix} \sqrt{1/3}\,|0\rangle & -\sqrt{2/3}\,|+\rangle \\ \sqrt{2/3}\,|-\rangle & -\sqrt{1/3}\,|0\rangle \end{pmatrix}$$

Spin 1 Chains

The AKLT Model: A prototypical Resonating Valence Bond groundstate

- $H = \sum_{<ij>} \left[\vec{S}_i \cdot \vec{S}_j + \beta (\vec{S}_i \cdot \vec{S}_j)^2 \right]$
- $\beta = 0$: usual Heisenberg spin chain
  - Haldane: unlike half-integer spin chains, integer spin chains have a gap
  - string order parameter: $S^z_0 \ \exp\left[i\pi \sum_{m=1}^{n-1} S^z_m \right] \ S^z_n \to$ constant
  - free Z_2 parameter at the boundary: effective spin-$1/2$ edge states
- $\beta = 1/3$: exactly solvable groundstate

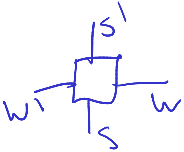
Matrix product realization:

- $A = \begin{pmatrix} \sqrt{1/3} & |0\rangle & -\sqrt{2/3} & |+\rangle \\ \sqrt{2/3} & |-\rangle & -\sqrt{1/3} & |0\rangle \end{pmatrix}$

Dont́ hard-code the Hamiltonian, use an MPO

$$\left(\tilde{I}' \quad \tilde{S}^{z\prime} \quad \tilde{S}^{+\prime} \quad \tilde{S}^{-\prime} \quad \tilde{H}'\right) =$$

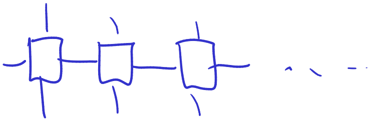
$$\left(\tilde{I} \quad \tilde{S}^{z} \quad \tilde{S}^{+} \quad \tilde{S}^{-} \quad \tilde{H}\right) \otimes \begin{pmatrix} I & S^z & S^+ & S^- & 0 \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & \frac{1}{2}S^- \\ 0 & 0 & 0 & 0 & \frac{1}{2}S^+ \\ 0 & 0 & 0 & 0 & I \end{pmatrix}$$

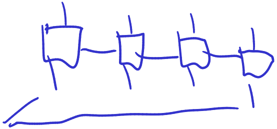


W x W matrix of
S x S local operators

MPO as a tensor

Hamiltonian operator





vectors of operators

Matrix Product Operators

IPM J. Stat. Mech. P10014 (2007), arXiv:0804.2509

- At each iteration we have a set of *block operators*, acting on the m-dimensional auxiliary space
- It is natural to use a Matrix Product approach to constructing the block operators used in DMRG

Ising model $H = \sum_{<i,j>} S_i^z S_j^z + \lambda \sum_i S_i^x$, adding a site to the block:

(identity operator)	I	$\rightarrow$	$I \otimes I_{\text{local}}$
(z-spin acting on right-most site)	S^z	$\rightarrow$	$I \otimes S^z_{\text{local}}$
(block Hamiltonian)	H	$\rightarrow$	$\lambda I \otimes S^x_{\text{local}} + S^z \otimes S^z_{\text{local}} + H \otimes I_{\text{local}}$

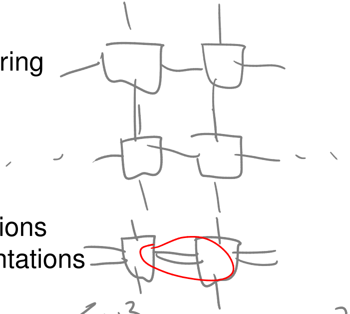
In matrix form:

$$\underbrace{\begin{pmatrix} I & S^z & H \end{pmatrix}'}_{\text{new block operators}} = \underbrace{\begin{pmatrix} I & S^z & H \end{pmatrix}}_{\text{old block operators}} \times \underbrace{\begin{pmatrix} I & S^z & \lambda S^x \\ & & S^z \\ & & I \end{pmatrix}}_{\text{local}}$$

Matrix Product Operators

This form can represent many operators

- fermionic $c^\dagger_{k=0}$: $W_{c^\dagger_{k=0}} = \begin{pmatrix} P & c^\dagger \\ & I \end{pmatrix}$, $P = (-1)^N$, J-W string
- finite momentum $b^\dagger_k$: $W_{b^\dagger_k} = \begin{pmatrix} e^{ik} & b^\dagger \\ & I \end{pmatrix}$



Advantages of the MPO representation: *arithmetic operations!*

$H_1 + H_2$	direct sum of the MPO representations
$H_1 \times H_2$	direct product of the MPO representations

$\langle H^2 \rangle - \langle H \rangle^2$

also derivatives, etc

This preserves the lower triangular form.

In the thermodynamic limit:

$$\langle A \rangle_L = \text{polynomial function of } L$$

Examples:

- Energy: $\langle H \rangle_L = L\,\epsilon$
- Hamiltonian block operator matrix elements to restart a calculation
- Single-mode approximation: $\langle S^-_k H S^+_k \rangle_L / \langle S^-_k S^+_k \rangle_L$