Density Matrix Renormalization Group Revisited (1)
Central Theorem — Optimal Low-Rank Density Matrix for a Block in Environment

6/16/03

Definitions

Superblock ($\mathcal{S}$) = a coupled block ($\mathcal{B}$) + environment ($\mathcal{E}$):

$$\mathcal{S} = \mathcal{B} \cup \mathcal{E} \tag{1}$$

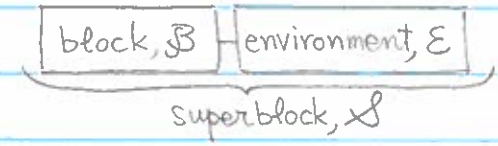
$$\mathcal{B} = \text{span}\{|i\rangle \,|\, i = 1, \ldots, N\} \tag{2}$$

$$\mathcal{E} = \text{span}\{|j\rangle \,|\, j = 1, \ldots, M\} \tag{3}$$

where $\{|i\rangle\}$ and $\{|j\rangle\}$ are orthonormal bases,

$$\langle i|i'\rangle = \delta_{ii'} \tag{4}$$

$$\langle j|j'\rangle = \delta_{jj'} \tag{5}$$



(Ground state)

$$|\psi\rangle = \sum_{i=1}^{N} \sum_{j=1}^{M} \psi_{ij} |i\rangle|j\rangle \tag{6}$$

(Reduced density matrix)

Consider an arbitrary operator A that operates only in $\mathcal{B}$. Its expectation value is obtained as

$$\langle A(\mathcal{B})\rangle = \sum_{i} \sum_{j} \langle j|\langle i|\psi_{ij}^{*} A(\mathcal{B}) \sum_{i'} \sum_{j'} \psi_{i'j'} |i'\rangle|j'\rangle$$

$$= \sum_{i} \sum_{i'} \sum_{j} \sum_{j'} \psi_{i'j'} \psi_{ij}^{*} \langle i|A(\mathcal{B})|i'\rangle \underbrace{\langle j|j'\rangle}_{\delta_{jj'}}$$

$$= \sum_{i} \sum_{i'} \underbrace{\left(\sum_{j} \psi_{i'j} \psi_{ij}^{*} \right)}_{\rho_{i'i}} \underbrace{\langle i|A(\mathcal{B})|i'\rangle}_{A_{ii'}}$$

$$\therefore \quad \langle A(\mathcal{B}) \rangle = \sum_{i=1}^{N} \sum_{i'=1}^{M} \rho_{ii'} A_{i'i} = tr_{\mathcal{B}}(\rho A) \tag{7}$$

where

$$\rho_{ii'} = \sum_{j=1}^{M} \psi_{ij} \psi^{*}_{i'j} \tag{8}$$

$$A_{i'i} = \langle i' | A(\mathcal{B}) | i \rangle \tag{9}$$

The reduced matrix $\rho_{ii'}$, which operates for a block in environment, is the central vehicle of DMRG.

— Problem

Optimal $\rho_{ii'}$ of rank-m ($\ll N$) ?

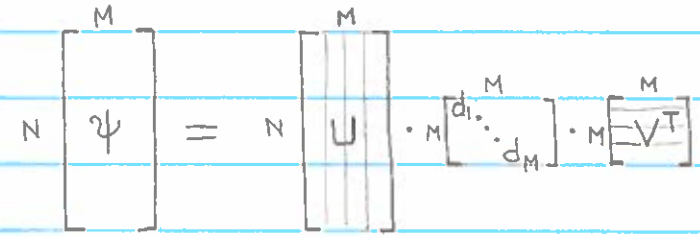
— Solution

Singular value decomposition (SVD) of ψ_{ij}

— Singular value decomposition

Let assume $N \geq M$. Otherwise, we can simply switch the role of N and M.

(Theorem) An $N \times M$ matrix Ψ ($N \geq M$) can be decomposed as



$$\Psi = U \cdot \begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_M \end{bmatrix} \cdot V^T \tag{10}$$

or

$$\underset{NM}{\Psi} = \underset{NM}{U}\,\underset{MM}{D}\,\underset{MM}{V^T} \tag{11}$$

where

$$D = \mathrm{diag}(d_1, \ldots, d_M) \tag{12}$$

$U = [u_i^{(\nu)}]$ is an $N \times M$ column orthogonal matrix

$$\sum_{i=1}^{N} u_i^{(\nu)} u_i^{(\nu')} = \sum_{i=1}^{N} U^T_{\nu i} U_{i\nu'} = \delta_{\nu\nu'} \tag{13}$$

or

$$U^T U = I_M \tag{14}$$

and $V = [v_j^{(\nu)}]$ is an $M \times M$ column orthogonal matrix

$$\sum_{j=1}^{M} v_j^{(\nu)} v_j^{(\nu')} = \sum_{j=1}^{M} V^T_{\nu j} V_{j\nu'} = \delta_{\nu\nu'} \tag{15}$$

or

$$V^T V = I_M \quad \text{(orthonormality)} \tag{16}$$

Since V is square, it is also row-orthogonal,

$$V V^T = I_M \quad \text{(completeness)} \tag{17}$$

or

$$\sum_{\nu=1}^{M} v_j^{(\nu)} v_{j'}^{(\nu)} = \delta_{jj'} \tag{18}$$

☺ (completeness)

Any vector $a \in \mathbb{R}^M$ can be expressed as a linear combination of M linearly-independent vectors,

$$a_i = \sum_{\nu=1}^{M} c_\nu v_i^{(\nu)}$$

$\sum_{i=1}^{M} v_i^{(\mu)} \times$ (above)

$$\sum_{i=1}^{M} v_i^{(\mu)} a_i = \sum_{\nu=1}^{M} c_\nu \underbrace{\sum_{i=1}^{M} v_i^{(\mu)} v_i^{(\nu)}}_{(V^T V)_{\mu\nu} = \delta_{\mu\nu}} = c_\mu$$

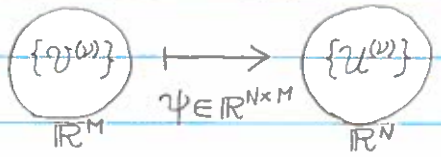
$$\therefore \forall a_i = \sum_{\nu=1}^{M} v_i^{(\nu)} \underbrace{\sum_{i'=1}^{M} v_{i'}^{(\nu)} a_{i'}}_{c_\nu}$$

$$= \sum_{i'=1}^{M} \underbrace{\left(\sum_{\nu=1}^{M} v_i^{(\nu)} v_{i'}^{(\nu)} \right)}_{\delta_{ii'}} a_{i'}$$

$$\therefore (VV^T)_{ii'} = \sum_{\nu=1}^{M} v_i^{(\nu)} v_{i'}^{(\nu)} = \delta_{ii'} \quad //$$

(Interpretation of SVD)

In SVD, $\Psi \in \mathbb{R}^{N\times M}$ maps an orthonormal basis $\{v^{(\nu)} \in \mathbb{R}^M\}$ onto another orthonormal basis $\{u^{(\nu)} \in \mathbb{R}^N\}$:



$$\Psi v^{(\nu)} = u^{(\nu)} d_\nu \qquad \text{(eigen-like relation)} \tag{19}$$

where

$$\begin{cases} v^{(\mu)T} v^{(\nu)} = \delta_{\mu\nu} \\ u^{(\mu)T} u^{(\nu)} = \delta_{\mu\nu} \end{cases} \qquad \text{(orthonormality)} \tag{20}$$

There can be at maximum M such relations, since there are only M linearly-independent vectors in $\mathbb{R}^M$.

— Low-rank approximation to $\rho_{ii'}$

(Theorem) Let $\Psi = UDV^T$ be the SVD of Ψ with the diagonal elements in descending order $d_1 \geq d_2 \geq \cdots \geq d_M$. Let

$$\underset{N\times M}{\Psi^{(m)}} = \sum_{\nu=1}^{m} \underset{N\times 1}{U^{(\nu)}} d_\nu \underset{1\times M}{V^{(\nu)T}} \tag{21}$$

be the rank-m truncation of the SVD. Then,

$$\min_{\text{rank}(A)=m} \|\Psi - A\|_2 = \|\Psi - \Psi^{(m)}\|_2 = d_{m+1} \tag{22}$$

where the matrix 2-norm $\|A\|_2 = \max_{\|x\|_2=1,\ x\in\mathbb{R}^M} \|Ax\|_{\mathbb{R}^N}$ is defined in terms of vector 2-norms.
(White used the Frobenius norm, $\|A\|_F = \sqrt{\sum_{ij} |a_{ij}|^2}$.)

Therefore, $\Psi^{(m)}$ is the optimal rank-m approximation to Ψ.

(Reduced density matrix)

Substituting the rank-m approximation Eq.(21) in Eq.(8),

$$\begin{aligned}
\underset{NM\ MN}{\rho} &= \Psi\,\Psi^T \\
&\simeq \sum_{\nu=1}^{m} U^{(\nu)} d_\nu V^{(\nu)T} \sum_{\nu'=1}^{m} V^{(\nu')} d_{\nu'} U^{(\nu')T} \\
&= \sum_{\nu}\sum_{\nu'} U^{(\nu)} d_\nu \underbrace{(V^{(\nu)T} V^{(\nu')})}_{\delta_{\nu\nu'}\ (\text{☺ orthogonality})} d_{\nu'} U^{(\nu')T} \\
&= \sum_{\nu=1}^{m} U^{(\nu)} d_\nu^2 U^{(\nu)T}
\end{aligned}$$

$$\therefore \rho \simeq \sum_{\nu=1}^{m} U^{(\nu)} w_\nu U^{(\nu)T} \tag{23}$$

or

$$\rho_{ii'} \simeq \sum_{\nu=1}^{m} U_i^{(\nu)} w_\nu U_{i'}^{(\nu)} \tag{24}$$

where

$$w_\nu = d_\nu^2 \tag{25}$$

(Sum rule)

$$\mathrm{Tr}\,\rho = \mathrm{Tr}\,\Psi\Psi^T = \mathrm{Tr}\,\Psi^T\Psi \tag{26}$$

Note that

$$\langle\Psi|\Psi\rangle = \sum_{ij}\langle j|\langle i|\Psi^*_{ij}\sum_{i'j'}\Psi_{i'j'}|i'\rangle|j'\rangle$$

$$= \sum_{ij}\sum_{i'j'}\underbrace{\langle j|j'\rangle}_{\delta_{jj'}}\underbrace{\langle i|i'\rangle}_{\delta_{ii'}}\Psi^*_{ij}\Psi_{i'j'}$$

$$= \sum_{ij}\Psi^*_{ij}\Psi_{ij} = \mathrm{Tr}\,\Psi^T\Psi = 1 \tag{27}$$

Therefore,

$$\mathrm{Tr}\,\rho = \mathrm{Tr}\,\Psi\Psi^T = 1 \tag{28}$$

Note that

$$\mathrm{Tr}\,\rho = \mathrm{Tr}\,\Psi\Psi^T$$

$$= \mathrm{Tr}\,UD\underbrace{V^TV}_{I_M}DU^T$$

$$= \mathrm{Tr}\,UD^2U^T$$

$$= \mathrm{Tr}\,\underbrace{U^TU}_{I_{MM}}D^2$$

$$= \mathrm{Tr}\,D^2 \tag{29}$$

Comparing Eqs. (28) and (29),

$$\mathrm{Tr}\,\rho = \sum_{\nu=1}^{M} d_\nu^2 = \sum_{\nu=1}^{M} w_\nu = 1 \tag{30}$$

(Summary)

The rank-m truncation of the SVD of the ground-state wavefunction,

$$\psi^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} d_\nu v^{(\nu)T} \tag{31}$$

or

$$\psi_{ij}^{(m)} = \sum_{\nu=1}^{m} u_i^{(\nu)} d_\nu v_j^{(\nu)} \tag{32}$$

produces the rank-m approximation to the reduced density matrix,

$$\rho^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} w_\nu u^{(\nu)T} \tag{33}$$

or

$$\rho_{ii'}^{(m)} = \sum_{\nu=1}^{m} u_i^{(\nu)} w_\nu u_{i'}^{(\nu)} \tag{34}$$

where

$$w_\nu = d_\nu^2 \tag{35}$$

The rank-m approximation $\rho^{(m)}$ is optimal in the least square sense with the error estimate,

$$\mathrm{Tr}(\rho - \rho^{(m)}) = 1 - \sum_{\nu=1}^{m} w_\nu \tag{36}$$

(Optimal reduced density matrix algorithm)

Given the superblock ground state $\psi_{ij} \in \mathbb{R}^{N \times M}$

1. Obtain the $N \times N$ reduced density matrix $\rho_{ii'} \in \mathbb{R}^{N \times M}$ by integrating out the environment variables,

$$\rho_{ii'} = \sum_{j=1}^{M} \psi_{ij} \psi^*_{i'j} \tag{37}$$

2. Perform the SVD of $\rho_{ii'}$

$$\rho_{ii'} = \sum_{\nu=1}^{N} u_i^{(\nu)} w_\nu u_{i'}^{(\nu)} \tag{38}$$

or

$$\rho = \sum_{\nu=1}^{N} u^{(\nu)} w_\nu u^{(\nu)T} \tag{39}$$

where $w_1 \geq w_2 \geq \cdots \geq w_N \geq 0$.

3. Retain only the first m terms in the expansion

$$\rho^{(m)}_{ii'} = \sum_{\nu=1}^{m} u_i^{(\nu)} w_\nu u_{i'}^{(\nu)} \tag{40}$$

or

$$\rho^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} w_\nu u^{(\nu)T} \tag{41}$$

Density Matrix Renormalization Group Revisited (2)
Greedy / Growth Algorithm

6/17/03

[S.R. White, Phys. Rev. B 48, 10345 ('93); S. Daul, I. Ciofini, C. Daul, S.R. White, Int'l J. Quantum Chem. 79, 331 ('00)]

— Objective

Obtain the ground state without diagonalizing a large matrix.

— Approach: Greedy / growth algorithm

Grow an incrementally larger block (cf. Dijkstra's shortest-path algorithm), for which the optimal constant low-rank (rank-m) approximation is known (greedy).

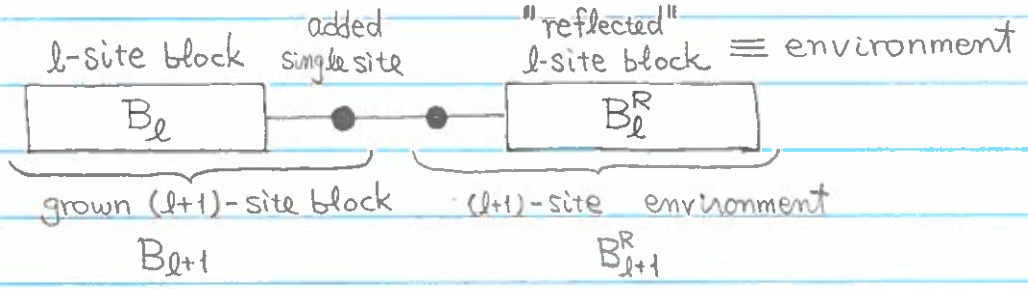
↑

By successively increasing the block size, while keeping the constant (m) rank for its density matrix:

{ i) Throw out higher excited states, which do not alter the ground state;

{ ii) Add low-energy perturbation to refine the constant (rank-m) size renormalized (dressed) basis.

— Block/environment construction for 1D system.



{ i) Reflected (right interchanged with left) block acts as environment.
ii) Growth achieved by adding a single site.

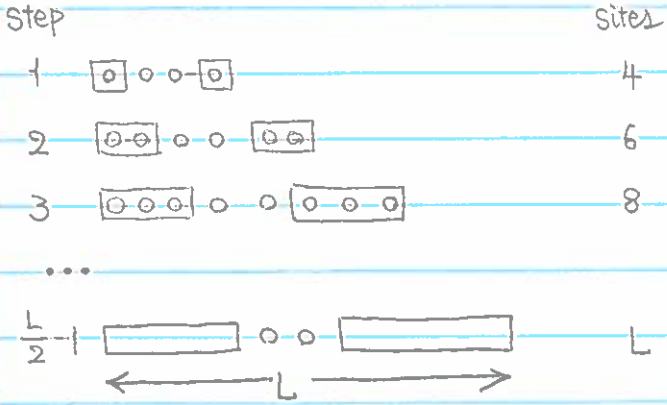
— Infinite system algorithm

Starting from a superblock-environment consisting 4 single sites, grow the superblock each time by adding a single site until the superblock-environment contains L sites after $(\frac{L}{2}-1)$ steps.

☺ $\underbrace{2(s-1)}_{\text{except for the 1st step, one added per step}} + \underbrace{4}_{\text{initially 4-site superblock + environment}} = L$

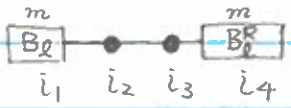
$\therefore \quad s-1+2 = \frac{L}{2}$

$\therefore \quad s = \frac{L}{2}-1$ //



1. Make four initial blocks, each consisting of a single site. Set up the block Hamiltonian.

2. Form the superblock Hamiltonian by adding cross terms.



3. Obtain the superblock ground state by the Davidson method,
$\psi(i_1, i_2, i_3, i_4)$
(Compute physical expectation values here.)

4. Form the reduced density (matrix) for the 1-2 block by integrating out the environment variables (3-4),

$$\rho(i_1, i_2; i_1', i_2') = \sum_{i_3, i_4} \psi(i_1, i_2, i_3, i_4)\, \psi^*(i_1', i_2', i_3, i_4)$$

5. Diagonalize ρ to find eigenvalues w_ν ($w_1 \geq w_2 \geq \cdots$) and eigenvectors $u^{(\nu)}_{i_1 i_2}$; discard all but m largest eigenvalues.

6. Form matrix representation of operators for the two-block (1-2) system, and form a new block 1 by changing basis to $u^{(\nu)}$: $H_1' = O\, H_{12}\, O^T$, where $O(\nu; i_1, i_2) = u^{(\nu)}_{i_1 i_2}$ (ν: m; i_1, i_2: $m_1 m_2$) (e.g. 1 site can add $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$ ~~degrees of freedom, and $m_1 m_2 = 4m$; $16m^2 \to m^2$ reduction~~).

7. Replace old block 1 with new block 1; replace old block 4 with the reflection of new block 1.

8. Go to step 2

- Lesson.

Block-enlarging perturbation (cf. Cuppen divide-and-conquer secular equation) should involve only renormalized/dressed (low-rank) operators — e.g. through Wannier orbitals without seeing real-space meshes / linear combination of Wannier functions.

↓

Local relaxation ⟷ reduced subspace diagonalization cycle?