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 ($\mathcal{E}$):

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

$$\mathcal{B} = \text{Span} \{ |i_i\rangle | i = 1, \ldots, N \}$$

$$\mathcal{E} = \text{Span} \{ |j_j\rangle | j = 1, \ldots, M \}$$

where $\{ |i_i\rangle \}$ and $\{ |j_j\rangle \}$ are orthonormal bases,

$$\langle i_i | i'_{i'} \rangle = \delta_{i,i'}$$

$$\langle j_j | j'_{j'} \rangle = \delta_{j,j'}$$

(Ground state)

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

(Reduced density matrix)

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

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

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

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

$$\rho_{ii} A_{ii'}$$
\[ \langle A(B) \rangle = \sum_{i=1}^{N} \sum_{i=1}^{M} P_{ii'} A_{ii'} = tr_{g}(\rho A) \]  
where
\[ P_{ii'} = \sum_{j=1}^{M} \Psi_{ij} \Psi_{i'j}^* \]

\[ A_{ii'} = \langle i' | A(B) | i \rangle \]

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

**Problem**

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

**Solution**

Singular value decomposition (SVD) of \( \Psi_{ij} \)
-- 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 \( \Psi \) \( (N \geq M) \) can be decomposed as

\[
\begin{bmatrix}
\Psi
\end{bmatrix}_N = \begin{bmatrix}
U
\end{bmatrix}_N \cdot \begin{bmatrix}
\begin{bmatrix}
\Psi_1 \\
\vdots \\
\Psi_M
\end{bmatrix}
\end{bmatrix}_M \cdot \begin{bmatrix}
V^T
\end{bmatrix}_M
\]

or

\[
\Psi = \begin{bmatrix}
\Psi_1 \\
\vdots \\
\Psi_M
\end{bmatrix}_M \cdot \begin{bmatrix}
U
\end{bmatrix}_N \cdot \begin{bmatrix}
\begin{bmatrix}
D_1 \\
\vdots \\
D_M
\end{bmatrix}
\end{bmatrix}_M \cdot \begin{bmatrix}
V^T
\end{bmatrix}_M
\]

where

\[ D = \text{diag} (d_1, \ldots, d_M) \]  

\[ U = [U_i^{(w)}] \text{ is an } N \times M \text{ column orthogonal matrix} \]

\[ \sum_{i=1}^{N} U_i^{(w)} U_i^{(w)\top} = \sum_{i=1}^{N} U_i^{(w)\top} U_i^{(w)} = \delta_{\nu\nu} \]  

or

\[ U^\top U = I_M \]  

and \( V = [V_j^{(w)}] \text{ is an } M \times M \text{ column orthogonal matrix} \)

\[ \sum_{j=1}^{M} V_j^{(w)} V_j^{(w)\top} = \sum_{j=1}^{M} V_j^{(w)\top} V_j^{(w)} = \delta_{\nu\nu} \]  

or

\[ V^\top V = I_M \text{ (orthonormality)} \]  

Since \( V \) is square, it is also row-orthogonal,

\[ V V^\top = I_M \text{ (completeness)} \]

or

\[ \sum_{\nu=1}^{M} V_{\nu}^{(w)} V_{\nu}^{(w)\top} = \delta_{jj} \]
Any vector \( \mathbf{a} \in \mathbb{R}^M \) can be expressed as a linear combination of \( M \) linearly-independent vectors,

\[
\mathbf{a}_i = \sum_{\nu=1}^{M} c_{\nu} \mathbf{v}^{(\nu)}_i
\]

\[
\sum_{i=1}^{M} \mathbf{v}^{(\nu)}_i \mathbf{a}_i = \sum_{\mu=1}^{M} c_{\nu} \left( \sum_{i=1}^{M} \mathbf{v}^{(\mu)}_i \mathbf{v}^{(\nu)}_i \right) = c_{\mu}
\]

\[
(\mathbf{V}^\mathbf{V})_{\mu\nu} = \delta_{\mu\nu}
\]

\[
\therefore \forall \mathbf{a}_i = \sum_{\nu=1}^{M} \mathbf{v}^{(\nu)}_i \left( \sum_{\mu=1}^{M} \mathbf{v}^{(\mu)}_i \mathbf{a}_i \right) = \sum_{i=1}^{M} \left( \sum_{\nu=1}^{M} \mathbf{v}^{(\nu)}_i \mathbf{a}_i \right) \mathbf{a}_i'
\]

\[
(\mathbf{V}^\mathbf{V})_{ii'} = \sum_{\nu=1}^{M} \mathbf{v}^{(\nu)}_i \mathbf{v}^{(\nu)}_i = \delta_{ii'}
\]
(Interpretation of SVD)

In SVD, \( \Psi \in \mathbb{R}^{N \times M} \) maps an orthonormal basis \( \{ \psi^{(w)} \in \mathbb{R}^M \} \) onto another orthonormal basis \( \{ \xi^{(w)} \in \mathbb{R}^N \} \):

\[
\Psi \psi^{(w)} = \xi^{(w)} \lambda, \quad \text{(eigen-like relation)} \tag{19}
\]

where

\[
\begin{align*}
\psi^{(w)\top} \psi^{(\nu)} &= \delta_{\mu \nu} \quad \text{(orthonormality)} \\
\xi^{(w)\top} \xi^{(\nu)} &= \delta_{\mu \nu}
\end{align*}
\tag{20}
\]

There can be at maximum \( M \) such relations, since there are only \( M \) linearly-independent vectors in \( \mathbb{R}^M \).
Low-rank approximation to $\Psi$

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

$$\Psi^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} d_{\nu} u^{(\nu)T}$$

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

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

where the matrix 2-norm $\|A\|_2 = \max_{\|x\|_2=1} \|Ax\|_2$ 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 $\Psi$.

(Reduced density matrix)

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

$$\rho = \Psi \Psi^T$$

$$= \sum_{\nu=1}^{m} u^{(\nu)} d_{\nu} u^{(\nu)T} \sum_{\nu=1}^{m} u^{(\nu)} d_{\nu} u^{(\nu)T}$$

$$= \sum_{\nu=1}^{m} u^{(\nu)} d_{\nu} \delta_{\nu \nu} (\Psi \Psi^T)$$

$$= \sum_{\nu=1}^{m} u^{(\nu)} d_{\nu}^2 u^{(\nu)T}$$

$$\therefore \rho \approx \sum_{\nu=1}^{m} u^{(\nu)} w_\nu \bar{u}^{(\nu)T}$$

or

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

where

$$w_\nu = d_{\nu}^2$$
(Sum rule)

\[ T_n \rho = T_n \psi \psi^T = T_n \psi \psi \]  

(26)

Note that

\[ <\psi|\psi> = \sum_{ij} \langle ii | \psi_{ij}^* \frac{\delta_{ij}}{\delta_{ij}} \psi_{ji} | jj> \]

\[ = \sum_{ij} \langle ii | \psi_{ij}^* \frac{\delta_{ij}}{\delta_{ij}} \psi_{ji} | jj> = T_n \psi \psi = 1 \]  

(27)

Therefore,

\[ T_n \rho = T_n \psi \psi^T = 1 \]  

(28)

Note that

\[ T_n \rho = T_n \psi \psi^T \]

\[ = T_n UD \psi U^T \]

\[ = T_n UD^2 U^T \]

\[ = T_n \frac{U^T \psi U}{I_{MM}} \]

\[ = T_n \psi \psi \]  

(29)

Comparing Eqs. (28) and (29),

\[ T_n \rho = \sum_{v=1}^{M} d_v^2 = \sum_{v=1}^{M} \omega_v = 1 \]  

(30)
The rank-\(m\) truncation of the SVD of the ground-state wavefunction,

\[
\phi_{\mu}^{(m)} = \sum_{\nu=1}^{m} U^{(\nu)} \psi_{\nu} \psi_{\nu}^{T} \tag{31}
\]

or

\[
\phi_{ij}^{(m)} = \sum_{\nu=1}^{m} U_{i}^{(\nu)} d_{\nu} \psi_{j}^{(\nu)} \tag{32}
\]

produces the rank-\(m\) approximation to the reduced density matrix,

\[
\rho^{(m)} = \sum_{\nu=1}^{m} U^{(\nu)} \psi_{\nu} \psi_{\nu}^{T} \tag{33}
\]

or

\[
\rho_{ii}^{(m)} = \sum_{\nu=1}^{m} U_{i}^{(\nu)} \psi_{\nu} \psi_{i}^{(\nu)} \tag{34}
\]

where

\[
\psi_{\nu} = d_{\nu}^{2} \tag{35}
\]

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

\[
\text{Tr}(\rho - \rho^{(m)}) = 1 - \sum_{\nu=1}^{m} \psi_{\nu} \tag{36}
\]
(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 $\rho_{ii'} \in \mathbb{R}^{N \times N}$ by integrating out the environment variables,

$$
\rho_{ii'} = \sum_{j=1}^{M} \psi_{ij} \psi_{ij}^* 
$$

(37)

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

$$
\rho_{ii'} = \sum_{\nu=1}^{N} \psi_{ii}(\nu) \psi_{ii}(\nu)^* 
$$

or

$$
\rho = \sum_{\nu=1}^{N} \psi(\nu) \psi(\nu)^* 
$$

(38)

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

3. Retain only the first $m$ terms in the expansion

$$
\rho_{ii'}^{(m)} = \sum_{\nu=1}^{m} \psi_{ii}(\nu) \psi_{ii}(\nu)^* 
$$

or

$$
\rho^{(m)} = \sum_{\nu=1}^{m} \psi(\nu) \psi(\nu)^* 
$$

(40)
Density Matrix Renormalization Group Revisited (2)
Greedy / Growth Algorithm 6/17/03


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:

1) Throw out higher excited states, which do not alter the ground state;
2) Add low-energy perturbation to refine the constant (rank-m) size renormalized basis.
(dressed)
Block/environment construction for 1D system:

\begin{align*}
  \text{l-site block} & \quad \text{added single site} & \quad \text{"reflected" l-site block} = \text{environment} \\
  B_l & \quad \text{grown (l+1)-site block} & \quad B_{l+1}^R \\
  B_{l+1} & \quad \text{(l+1)-site environment} & \quad B_{l+1}^R
\end{align*}

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

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Infinite system algorithm

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

\[ 2(s-1) + 4 = L \]

\[ \text{except for the initially added per sup superblock+environment} \]

\[ \therefore S = 1 + 2 = \frac{L}{2} \]

\[ \therefore S = \frac{L}{2} - 1 \]

\[ \text{Step} \quad \text{Sites} \]
\[ 1 \quad 4 \]
\[ 2 \quad 6 \]
\[ 3 \quad 8 \]
\[ \vdots \]
\[ \frac{L}{2} - 1 \quad L \]
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),

   \[ P(i_1, i_2; i'_1, i'_2) = \sum_{i_3, i_4} \Psi(i_1, i_2, i_3, i_4) \Psi^*(i'_1, i'_2, i_3, i_4) \]

5. Diagonalize \( P \) to find eigenvalues \( \lambda_j \) \((1, 2, \lambda_2, \ldots)\) and eigenvectors \( \Psi_{i_1i_2}^{(v)} \); 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 \( U^{(v)} \):

   \[ H_1' = U H_2 U^T \]

   where \( U(i_1, i_2) = U^{(v)}_{i_1i_2} \) (e.g. 1 site can add \( m \) \( m' \) \( m'' \) \( m'' \) \( m'' \) \( m'' \) degrees of freedom, and \( m, m' = 4m', 16m' \rightarrow m^2 \) 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.

\[ \text{Local relaxation} \rightarrow \text{reduced subspace diagonalization cycle?} \]