**Singular Value Decomposition: Reduced Density Matrix**

We will introduce the singular value decomposition of a matrix in the context of the reduced density matrix of a quantum system connected to an environment.

**REDUCED DENSITY MATRIX**

Let us consider a quantum system (block) $B$, which is spanned by the $N$-dimensional orthonormal basis set $\{|i\rangle \mid i = 1, \ldots, N\}$, surrounded by an environment $E$, which is spanned by the $M$-dimensional orthonormal basis set $\{|j\rangle \mid j = 1, \ldots, M\}$ (see the figure below).

![Diagram of block and environment](image)

The ground state of the total (= block + environment) system can be represented as

$$|\psi\rangle = \sum_{i=1}^{N} \sum_{j=1}^{M} \psi_{ij} |i\rangle |j\rangle.$$  \hspace{1cm} (1)

Now consider the expectation value of an arbitrary operator, $A$, which acts only within the block:

$$\langle A \rangle = \sum_{i} \sum_{j} \sum_{i'} \sum_{j'} \psi_{ij}^* \langle j|A|i'\rangle \psi_{i'j'} |j\rangle |i\rangle,$$

$$= \sum_{i} \sum_{j} \sum_{i'} \sum_{j'} \sum_{i''} \psi_{ij}^* \psi_{i''j''} \langle i|A|i''\rangle \langle j'\rangle |i'\rangle,$$

$$= \sum_{i} \sum_{i'} \sum_{j} \psi_{ij}^* \psi_{i'j} \langle i|A|i'\rangle,$$

$$= \sum_{i} \sum_{i'} \rho_{ii'} A_{i'i'} = \text{tr}_B(\rho A),$$  \hspace{1cm} (2)

where the reduced density matrix is defined as

$$\rho_{ii'} = \sum_{j} \psi_{ij}^* \psi_{i'j},$$  \hspace{1cm} (3)

and the matrix element of the operator is $A_{i'i''} = \langle i|A|i''\rangle$.

**SINGULAR VALUE DECOMPOSITION (SVD)**

**Problem**: What is the optimal reduced density matrix $\rho$ of rank-$m$ ($<< N$)?

**Solution**: Singular value decomposition (SVD) of $\psi \in \mathbb{R}^N \times \mathbb{R}^M$.

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

$$\begin{bmatrix} \psi \\ \end{bmatrix} = \begin{bmatrix} U \\ \end{bmatrix} \begin{bmatrix} d_1 & \cdots \\ \vdots \\ d_M \\ \end{bmatrix} \begin{bmatrix} V^T \\ \end{bmatrix},$$  \hspace{1cm} (4)

or

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\[ \psi = UDV^T, \]  
(5)

where \( U = \left[ U_{iv} = u_{i}^{(v)} \right] \in \mathbb{R}^N \times \mathbb{R}^M \) is column orthogonal, i.e.,

\[ \sum_{i=1}^{N} u_{i}^{(v)} u_{i}^{(v')} = \delta_{v,v'}, \]  
(6)

or

\[ U^T U = I_M, \]  
(7)

and \( V = \left[ V_{iv} = v_{i}^{(v)} \right] \in \mathbb{R}^M \times \mathbb{R}^M \) is column orthogonal, i.e.,

\[ \sum_{i=1}^{M} v_{i}^{(v)} v_{i}^{(v')} = \delta_{v,v'}, \]  
(8)

or

\[ V^T V = I_M. \]  
(9)

The columns of \( U \), whose same-numbered elements \( d_v \) are nonzero, are an orthonormal set of basis vectors that span the range (see Appendix for the range); the columns of \( V \), whose same-numbered elements \( d_v \) are zero, are an orthonormal basis for the nullspace that is mapped to zero, i.e., the subspace of \( x \in \mathbb{R}^M \), where \( \psi x = 0 \). The program, singular.c, in the source code directory of the class home page demonstrates this automatic construction of orthonormal bases for the range and the nullspace.

**TRUNCATED SVD AS OPTIMAL APPROXIMATION**

(Theorem) Let \( \psi = UDV^T \) be the SVD of \( \psi \) with the diagonal elements in descending order \( d_1 \geq d_2 \geq \ldots \geq d_M \), and let

\[ \psi^{(m)} = \sum_{v=1}^{m} u_{i}^{(v)} d_v v_{i}^{(v)} T, \]  
(10)

be the rank-\( m \) truncation of the SVD. Then

\[ \min_{\text{rank}(A)=m} \| A - \psi \|_2 = \| \psi^{(m)} - \psi \|_2 = d_{m+1}, \]  
(11)

where the matrix 2-norm is defined in terms of the vector 2-norm as \( \| A \|_2 = \min_{\| x \|_2 = 1} \| Ax \|_2 \). Therefore, \( \psi^{(m)} \) is the optimal rank-\( m \) approximation to \( \psi \).

Equation (10) shows that SVD is a representation of a matrix as a sum of outer products of two vectors, just as a density matrix is.

**LOW-RANK APPROXIMATION TO THE REDUCED DENSITY MATRIX**

Substituting the rank-\( m \) approximation (10) in the definition of the reduced density matrix, Eq. (3),
\[ \rho = \psi \psi^T \]
\[ = \sum_{v=1}^{m} \sum_{v'=1}^{m} u_v^{(v)} d_v \left( \psi_v^{T} \right) \left( v' \right) d_v' u_{v'} \left( v' \right)^T \]
\[ = \sum_{v=1}^{m} \sum_{v'=1}^{m} u_v^{(v)} d_v \left( \delta_{v v'} \right) d_v u_{v'} \left( v' \right)^T \]
\[ = \sum_{v=1}^{m} u_v^{(v)} d_v^2 u_{v'} \left( v' \right)^T \]

(12)

(Summary) The rank-\( m \) truncation of the SVD of the global (= block + environment) ground state wave function,

\[ \psi^{(m)} = \sum_{v=1}^{m} u_v^{(v)} v^{(v) T} \]

or

\[ \psi_{ij}^{(m)} = \sum_{v=1}^{m} u_i^{(v)} v_{j}^{(v)} \]

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

\[ \rho^{(m)} = \sum_{v=1}^{m} u_v^{(v)} w_v u_{v'} \left( v' \right)^T \]

or

\[ \rho_{ii'}^{(m)} = \sum_{v=1}^{m} u_i^{(v)} w_v u_{i'} \left( v' \right) \]

where \( w_v = d_v^2 \). The rank-\( m \) approximation \( \rho^{(m)} \) is optimal in the least square sense.

**DENSITY MATRIX RENORMALIZATION GROUP**

The density matrix renormalization group (DMRG) algorithm by Steven White\(^2\) is a systematic procedure to accurately obtain a quantum ground state with a modest computational cost. The DMRG incrementally add environments to the block, solve the global (= block + environment) ground state, and construct a low-rank block density matrix to represent the block with reduced degrees of freedom.

**APPENDIX—RANK OF A MATRIX**

For an \( N \times M \) matrix \( A \), consider the mapping,

\[ x \left( \in \mathbb{R}^M \right) \xrightarrow{A} b = Ax \left( \in \mathbb{R}^N \right). \]

(A1)

The range of matrix \( A \) is the vector space spanned by all linearly independent vectors \( \{b\} \), which are mapped from some \( x \). The rank of matrix \( A \) is the size (i.e., the number of linearly independent vectors) of its range.