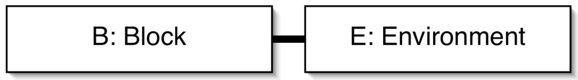
Singular Value Decomposition: Reduced Density Matrix

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[1]

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



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

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

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

$$\begin{aligned}\langle A\rangle &= \sum_i \sum_j \psi_{ij}^* \langle j|\langle i|A \sum_{i'} \sum_{j'} \psi_{i'j'}|i'\rangle|j'\rangle \\ &= \sum_i \sum_j \sum_{i'} \sum_{j'} \psi_{i'j'}\psi_{ij}^* \langle i|A|i'\rangle\langle j|j'\rangle \\ &= \sum_i \sum_{i'} \sum_j \psi_{i'j}\psi_{ij}^* \langle i|A|i'\rangle \\ &\equiv \sum_i \sum_{i'} \rho_{i'i} A_{ii'} = \mathrm{tr}_B(\rho A)\end{aligned}, \tag{2}$$

where the reduced density matrix is defined as

$$\rho_{i'i} \equiv \sum_j \psi_{i'j}\psi_{ij}^*, \tag{3}$$

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

SINGULAR VALUE DECOMPOSITION (SVD)

Problem: What is the optimal reduced density matrix ρ of rank-m ($\ll N$)?

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

(Theorem) An $N\times M$ matrix ψ (assume $N \geq M$) can be decomposed as (see Appendix A for proof of SVD and associated polar decomposition)

$$\begin{bmatrix} & & \\ & \psi & \\ & & \end{bmatrix} = \begin{bmatrix} & & \\ & U & \\ & & \end{bmatrix} \begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_M \end{bmatrix} \begin{bmatrix} & V^T & \end{bmatrix}, \tag{4}$$

or

$$\psi = UDV^T, \tag{5}$$

where $U = \left[U_{i\nu} = u_i^{(\nu)}\right] \in \mathbf{R}^N \times \mathbf{R}^M$ is column orthogonal, *i.e.*,

$$\sum_{i=1}^{N} u_i^{(\nu)} u_i^{(\nu')} = \delta_{\nu\nu'}, \tag{6}$$

or

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[1] R. P. Feynman, *Statistical Mechanics* (Benjamin/Cummings, Reading, MA, 1972) Chap. 2.

$$U^T U = I_M, \tag{7}$$

and $V = \left[V_{i\nu} = v_i^{(\nu)}\right] \in \mathbf{R}^M \times \mathbf{R}^M$ is column orthogonal, *i.e.*,

$$\sum_{i=1}^{M} v_i^{(\nu)} v_i^{(\nu')} = \delta_{\nu\nu'}, \tag{8}$$

or

$$V^T V = I_M. \tag{9}$$

The columns of U, whose same-numbered elements d_ν are *nonzero*, are an orthonormal set of basis vectors that span the range (see Appendix B for the range); the columns of V, whose same-numbered elements d_ν are *zero*, are an orthonormal basis for the nullspace that is mapped to zero, *i.e.*, the subspace of $x \in \mathbf{R}^M$, 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 ψ with the diagonal elements in descending order $d_1 \geq d_2 \geq \cdots \geq d_M$ and let

$$\psi^{(m)} \equiv \sum_{\nu=1}^{m} u^{(\nu)} d_\nu v^{(\nu)T}, \tag{10}$$

be the rank-m truncation of the SVD. Then

$$\min_{\mathrm{rank}(A)=m} \|A - \psi\|_2 = \left\|\psi^{(m)} - \psi\right\|_2 = d_{m+1}, \tag{11}$$

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

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),

$$\begin{aligned} \rho &= \psi\psi^T \\ &= \sum_{\nu=1}^{m} \sum_{\nu'=1}^{m} u^{(\nu)} d_\nu \left(v^{(\nu)T} v^{(\nu')}\right) d_{\nu'} u^{(\nu')T} \\ &= \sum_{\nu=1}^{m} \sum_{\nu'=1}^{m} u^{(\nu)} d_\nu (d_{\nu\nu'}) d_{\nu'} u^{(\nu')T} \\ &= \sum_{\nu=1}^{m} u^{(\nu)} d_\nu^2 u^{(\nu)T} \end{aligned}. \tag{12}$$

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

$$\psi^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} d_\nu v^{(\nu)T}, \tag{13}$$

or

$$\psi_{ij}^{(m)} = \sum_{\nu=1}^{m} u_{i^{(\nu)}} d_\nu v_{j^{(\nu)}}, \tag{14}$$

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

$$\rho^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} w_\nu u^{(\nu)T}, \tag{15}$$

or

$$\rho_{ii'}^{(m)} = \sum_{\nu=1}^{m} u_{i(\nu)} w_\nu u_{i'(\nu)}, \tag{16}$$

where $w_\nu = d_\nu^2$. 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 A — Polar and Singular-Value Decompositions

A.1 POLAR DECOMPOSITION

(Theorem) Let **A** be a real $N \times M$ matrix, where $N \geq M$ (*i.e.*, mapping from an *M*-dimensional source vector space to a larger *N*-dimensional target vector space). Then, there exists a column-wise orthogonal matrix **S** ($\in \Re^{N \times M}$ and) such that

$$\mathbf{A} = \mathbf{SJ}, \tag{A1}$$

$$\mathbf{S}^{\mathrm{T}}\mathbf{S} = \mathbf{I}^{M \times M}, \tag{A2}$$

where $\mathbf{I}^{M \times M}$ is the identity matrix and the unique nonnegative matrix **J** is

$$\mathbf{J} = \sqrt{\mathbf{A}^{\mathrm{T}}\mathbf{A}} \in \Re^{M \times M}. \tag{A3}$$

(Proof) Consider a spectral (or eigen) decomposition of **J**:

$$\mathbf{J} = \sum_{i=1}^{M} \lambda_i |i\rangle\langle i|, \tag{A4}$$

where $\lambda_i\ (\geq 0)$ is the i-th eigenvalue and $\{|i\rangle \in \Re^M \mid i = 1, \dots, M\}$ is an orthonormal set of eigenvectors, where $\langle i|j\rangle = \delta_{i,j}$. Define a mapped *N*-element vector

$$|\psi_i\rangle = \mathbf{A}|i\rangle\ (\in \Re^N), \tag{A5}$$

then

$$\langle\psi_i|\psi_j\rangle = \langle i|\mathbf{A}^{\mathrm{T}}\mathbf{A}|j\rangle = \langle i|\mathbf{J}^2|j\rangle = \lambda_j^2\langle i|j\rangle = \lambda_j^2\delta_{i,j}\ . \tag{A6}$$

For those eigenvectors with $\lambda_i \neq 0$, define

$$|e_i\rangle = |\psi_i\rangle/\lambda_i\ (\in \Re^N), \tag{A7}$$

so that these vectors are orthonormal, *i.e.*, $\langle e_i|e_j\rangle = \delta_{i,j}$. For those eigenvectors with $\lambda_i = 0$, we use the Gram-Schmidt procedure to construct an orthonormal basis set and append it to the above basis set. Define a column-wise orthogonal matrix,

$$\mathbf{S} = \sum_{i=1}^{M} |e_i\rangle\langle i| \in \Re^{N \times M} \tag{A8}$$

(note $\mathbf{S}^{\mathrm{T}}\mathbf{S} = \sum_{i=1}^{M}|i\rangle\langle e_i| \sum_{j=1}^{M}|e_j\rangle\langle j| = \sum_{i=1}^{M}\sum_{j=1}^{M}|i\rangle \underbrace{\langle e_i|e_j\rangle}_{\delta_{ij}} \langle j| = \sum_{i=1}^{M}|i\rangle\langle i| = \mathbf{I}^{M \times M}$.) When $\lambda_i \neq 0$, we have

$$\mathbf{SJ}|i\rangle = \sum_{j=1}^{M}|e_j\rangle\lambda_i \underbrace{\langle j|i\rangle}_{\delta_{ji}} = \lambda_i|e_i\rangle = |\psi_i\rangle = \mathbf{A}|i\rangle. \tag{A9}$$

When $\lambda_i = 0$,

$$\mathbf{SJ}|i\rangle = \sum_{j=1}^{M}|e_j\rangle \underbrace{\lambda_i}_{0} \underbrace{\langle j|i\rangle}_{\delta_{ji}} = 0|e_i\rangle = 0 = |\psi_i\rangle = \mathbf{A}|i\rangle. \tag{A10}$$

Namely, **SJ** is identical to **A** as a mapping for the entire *M*-dimensional source vector space. //

[2] S. R. White, "Density-matrix algorithms for quantum renormalization groups," *Physical Review B* **48**, 10345 (1993).

A.2 SINGULAR VALUE DECOMPOSITION

(Theorem) Let **A** be a real $N \times M$ matrix, where $N \geq M$ as above. Then, there exists column-wise orthogonal matrices **U** ($\in \Re^{N\times M}$) and **V** ($\in \Re^{M\times M}$), such that

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^{\mathrm{T}}, \tag{A11}$$

$$\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}^{M\times M}, \tag{A12}$$

where **D** ($\in \Re^{M\times M}$) is a nonnegative diagonal matrix.

(Proof) Consider the polar decomposition, **A** = **SJ**, in Eq. (A1). We perform the eigen-decomposition of **J** as

$$\mathbf{J} = \mathbf{V}\mathbf{D}\mathbf{V}^{\mathrm{T}}, \tag{A13}$$

where **D** is the diagonal matrix such that its matrix elements are

$$D_{ij} = \lambda_i \delta_{ij}, \tag{A14}$$

and **V** ($\in \Re^{M\times M}$) is an orthogonal matrix, *i.e.*, $\mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}^{M\times M}$. Substituting Eq. (A13) in Eq. (A1), we have

$$\mathbf{A} = \mathbf{S}\mathbf{V}\mathbf{D}\mathbf{V}^{\mathrm{T}} \equiv \mathbf{U}\mathbf{D}\mathbf{V}^{\mathrm{T}}, \tag{A15}$$

Note that **U** = **SV** ($\in \Re^{N\times M}$) is a column-wise orthogonal, since

$$\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{V}^{\mathrm{T}}\mathbf{S}^{\mathrm{T}}\mathbf{S}\mathbf{V} = \mathbf{V}^{\mathrm{T}}\underbrace{\mathbf{S}^{\mathrm{T}}\mathbf{S}}_{\mathbf{I}^{M\times M}}\mathbf{V} = \mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}^{M\times M}. //$$

Appendix B — Rank and Range of a Matrix

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

$$x(\in R^M) \underset{A}{\rightarrow} b = Ax(\in R^N). \tag{B1}$$

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.