Schmidt decomposition and entanglement

The Schmidt decomposition considers whether two subsystems A and B of a pure composite system AB are entangled or product states. The decomposition employs singular value decomposition to facilitate the task and affirm the reduced density operator test of entanglement, $tr\left(\left(\rho^A\right)^2\right) = tr\left(\left(\rho^B\right)^2\right) < 1$.

Theorem: Suppose $|\psi\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $|i_A\rangle$ for system A, and orthonormal states $|i_B\rangle$ of system B such that

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle$$

where λ_i are non-negative real numbers called Schmidt coefficients that satisfy $\sum_i \lambda_i^2 = 1$.

An implication of the Schmidt decomposition is that the reduced density operators are $\rho^A = \sum_i \lambda_i^2 |i_A\rangle \langle i_A|$ and $\rho^B = \sum_i \lambda_i^2 |i_B\rangle\langle i_B|$. In other words, their eigenvalues are the same, λ_i^2. If the number of positive eigenvalues, the Schmidt number, exceeds one then the two subsystems A and B are entangled; otherwise, they are tensor product subsystems. Further, if the subsystems are entangled then both reduced density operators are mixed states and have the same positive von Neumann (quantum) entropy. The pure state $|\psi\rangle$ has zero von Neumann entropy.

Construction.

Create an m x n matrix α from $|\psi\rangle$ where the elements of $|\psi\rangle$ are entered in the rows in order, m equals 2^a, n equals 2^b, a and b are the number of qubits in subsystem A and B, respectively. Construct the singular value decomposition of $\alpha = udv^T$ where u is m x r, d is r x r, v^T is r x n, the columns of u and v are orthonormal, d is a diagonal matrix of non-negative eigenvalues (the Schmidt coefficients), and r is the minimum of m and n.

The reduced density operators can be constructed from the singular value decomposition of α. $\rho^A = ud^2u^T$ and $\rho^B = vd^2v^T$. This is equivalent to applying the partial trace to recover the reduced density operators $\rho^A = tr_B\left(\rho^{AB}\right)$ and $\rho^B = tr_A\left(\rho^{AB}\right)$ where

$$tr_B\left(\rho^{AB}\right) = tr_B\left(|a_1\rangle \langle a_2| \otimes |b_1\rangle \langle b_2|\right) = |a_1\rangle \langle a_2| \, tr\left(|b_1\rangle \langle b_2|\right)$$

and $tr\left(|b_1\rangle\langle b_2|\right) = \langle b_2|b_1\rangle$. The two reduced density operators have the same eigenvalues and the Schmidt number indicates whether the subsystems A and B are entangled or product components.

Example.

Suppose the pure state is $|\psi\rangle = |\phi\rangle \otimes |+\rangle$ where $|\phi\rangle = 0.5830952\,|00\rangle + 0.5\,|01\rangle + 0.5\,|10\rangle + 0.4\,|11\rangle$ and $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Let system A refer to the first qubit and system B the last two qubits. Then,

$$\alpha = \begin{bmatrix} 0.4123106 & 0.4123106 & 0.3535534 & 0.3535534 \\ 0.3535534 & 0.3535534 & 0.2828427 & 0.2828427 \end{bmatrix}$$

Singular value decomposition of $\alpha = udv^T$ yields

$$u = \begin{bmatrix} 0.7681475 & -0.6402729 \\ 0.6402729 & 0.7681475 \end{bmatrix}$$

$$d = \begin{bmatrix} 0.99985947 & 0 \\ 0 & 0.01676428 \end{bmatrix}$$

and

$$v^T = \begin{bmatrix} 0.5431623 & 0.5431623 & 0.4527413 & 0.4527413 \\ 0.4527413 & 0.4527413 & -0.5431623 & -0.5431623 \end{bmatrix}$$

Hence, the Schmidt number is two indicating $|\phi\rangle$ is entangled and accessing only the first or second of its qubits creates uncertainty or von Neumann entropy.

This is further reinforced by examining the reduced density operators and their spectrum.

$$\rho^A = ud^2u^T = \begin{bmatrix} 0.59 & 0.4915476 \\ 0.4915476 & 0.41 \end{bmatrix}$$

and

$$\rho^B = vd^2v^T = \begin{bmatrix} 0.295 & 0.295 & 0.2457738 & 0.2457738 \\ 0.295 & 0.295 & 0.2457738 & 0.2457738 \\ 0.2457738 & 0.2457738 & 0.205 & 0.205 \\ 0.2457738 & 0.2457738 & 0.205 & 0.205 \end{bmatrix}$$

Importantly, the nonzero eigenvalues of ρ^B are identical to the eigenvalues of ρ^A. Hence, von Neumann entropy is the same for both systems A and B, $s\left(\rho^A\right) = s\left(\rho^B\right) = -\sum_i d_i \log d_i = 0.002579077$.

Singular value decomposition (svd) of $\alpha = udv^T = d_1 |u_1\rangle \langle v_1| + d_2 |u_2\rangle \langle v_2| =$

$$d_1 \begin{bmatrix} u_{11}v_{11} & u_{11}v_{12} & u_{11}v_{13} & u_{11}v_{14} \\ u_{12}v_{11} & u_{12}v_{12} & u_{12}v_{13} & u_{12}v_{14} \end{bmatrix} +$$

$$d_2 \begin{bmatrix} u_{21}v_{21} & u_{21}v_{22} & u_{21}v_{23} & u_{21}v_{24} \\ u_{22}v_{21} & u_{22}v_{22} & u_{22}v_{23} & u_{22}v_{24} \end{bmatrix} =$$

$$\begin{bmatrix} d_1u_{11}v_{11} + d_2u_{21}v_{21} & d_1u_{11}v_{12} + d_2u_{21}v_{22} & d_1u_{11}v_{13} + d_2u_{21}v_{23} & d_1u_{11}v_{14} + d_2u_{21}v_{24} \\ d_1u_{12}v_{11} + d_2u_{22}v_{21} & d_1u_{12}v_{12} + d_2u_{22}v_{22} & d_1u_{12}v_{13} + d_2u_{22}v_{23} & d_1u_{12}v_{14} + d_2u_{22}v_{24} \end{bmatrix}$$

svd also supplies the components to the theorem $|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle$. Let $\lambda_i = d_i$, $|i_A\rangle = |u_i\rangle$, and $|i_B\rangle = |v_i\rangle$. Then, $|\psi\rangle = d_1 |u_1\rangle |v_1\rangle + d_2 |u_2\rangle |v_2\rangle =$

$$d_1 \begin{bmatrix} u_{11}v_{11} \\ u_{11}v_{12} \\ u_{11}v_{13} \\ u_{11}v_{14} \\ u_{12}v_{11} \\ u_{12}v_{12} \\ u_{12}v_{13} \\ u_{12}v_{14} \end{bmatrix} + d_2 \begin{bmatrix} u_{21}v_{21} \\ u_{21}v_{22} \\ u_{21}v_{23} \\ u_{21}v_{24} \\ u_{22}v_{21} \\ u_{22}v_{22} \\ u_{22}v_{23} \\ u_{22}v_{24} \end{bmatrix} = \begin{bmatrix} d_1u_{11}v_{11} + d_2u_{21}v_{21} \\ d_1u_{11}v_{12} + d_2u_{21}v_{22} \\ d_1u_{11}v_{13} + d_2u_{21}v_{23} \\ d_1u_{11}v_{14} + d_2u_{21}v_{24} \\ d_1u_{12}v_{11} + d_2u_{22}v_{21} \\ d_1u_{12}v_{12} + d_2u_{22}v_{22} \\ d_1u_{12}v_{13} + d_2u_{22}v_{23} \\ d_1u_{12}v_{14} + d_2u_{22}v_{24} \end{bmatrix}$$

Variation.

On the other hand, if system A is the first two qubits and system B the third qubit, $|\phi\rangle$ and $|+\rangle$ are clearly product states and not entangled. The Schmidt construction is as follows.

$$\alpha = \begin{bmatrix} 0.4123106 & 0.4123106 \\ 0.3535534 & 0.3535534 \\ 0.3535534 & 0.3535534 \\ 0.2828427 & 0.2828427 \end{bmatrix}$$

Singular value decomposition of α is

$$u = \begin{bmatrix} 0.5830952 & 0.5 \\ 0.5 & -0.8420815 \\ 0.5 & 0.1579185 \\ 0.4 & 0.1263348 \end{bmatrix}$$

$$d = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

and

$$v^T = \begin{bmatrix} 0.7071068 & 0.7071068 \\ 0.7071068 & -0.7071068 \end{bmatrix}$$

The reduced density operators for systems A and B are

$$\rho^A = ud^2u^T = \begin{bmatrix} 0.34 & 0.2915476 & 0.2915476 & 0.2332381 \\ 0.2915476 & 0.25 & 0.25 & 0.2 \\ 0.2915476 & 0.25 & 0.25 & 0.2 \\ 0.2332381 & 0.2 & 0.2 & 0.16 \end{bmatrix}$$

and

$$\rho^B = vd^2v^T = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$$

As systems A and B are tensor products (not entangled), the Schmidt number is one and von Neumann (quantum) entropy is $s\left(\rho^A\right) = s\left(\rho^B\right) = 0$.

Singular value decomposition (svd) of $\alpha = udv^T = d_1 \left|u_1\right\rangle \left\langle v_1\right| + d_2 \left|u_2\right\rangle \left\langle v_2\right| =$

$$d_1 \begin{bmatrix} u_{11}v_{11} & u_{11}v_{12} \\ u_{12}v_{11} & u_{12}v_{12} \\ u_{13}v_{11} & u_{13}v_{12} \\ u_{14}v_{11} & u_{14}v_{12} \end{bmatrix} + d_2 \begin{bmatrix} u_{21}v_{21} & u_{21}v_{22} \\ u_{22}v_{21} & u_{22}v_{22} \\ u_{23}v_{21} & u_{23}v_{22} \\ u_{24}v_{21} & u_{24}v_{22} \end{bmatrix} =$$

$$\begin{bmatrix} d_1u_{11}v_{11} + d_2u_{21}v_{21} & d_1u_{11}v_{12} + d_2u_{21}v_{22} \\ d_1u_{12}v_{11} + d_2u_{22}v_{21} & d_1u_{12}v_{12} + d_2u_{22}v_{22} \\ d_1u_{13}v_{11} + d_2u_{23}v_{21} & d_1u_{13}v_{12} + d_2u_{23}v_{22} \\ d_1u_{14}v_{11} + d_2u_{24}v_{21} & d_1u_{14}v_{12} + d_2u_{24}v_{22} \end{bmatrix}$$

svd again supplies the components to the theorem $\left|\psi\right\rangle = \sum_i \lambda_i \left|i_A\right\rangle \left|i_B\right\rangle$. Let $\lambda_i = d_i$, $\left|i_A\right\rangle = \left|u_i\right\rangle$, and $\left|i_B\right\rangle = \left|v_i\right\rangle$. Then, $\left|\psi\right\rangle = d_1 \left|u_1\right\rangle \left|v_1\right\rangle + d_2 \left|u_2\right\rangle \left|v_2\right\rangle =$

$$d_1 \begin{bmatrix} u_{11}v_{11} \\ u_{11}v_{12} \\ u_{12}v_{11} \\ u_{12}v_{12} \\ u_{13}v_{11} \\ u_{13}v_{12} \\ u_{14}v_{11} \\ u_{14}v_{12} \end{bmatrix} + d_2 \begin{bmatrix} u_{21}v_{21} \\ u_{21}v_{22} \\ u_{22}v_{21} \\ u_{22}v_{22} \\ u_{23}v_{21} \\ u_{23}v_{22} \\ u_{24}v_{21} \\ u_{24}v_{22} \end{bmatrix} = \begin{bmatrix} d_1u_{11}v_{11} + d_2u_{21}v_{21} \\ d_1u_{11}v_{12} + d_2u_{21}v_{22} \\ d_1u_{12}v_{11} + d_2u_{22}v_{21} \\ d_1u_{12}v_{12} + d_2u_{22}v_{22} \\ d_1u_{13}v_{11} + d_2u_{23}v_{21} \\ d_1u_{13}v_{12} + d_2u_{23}v_{22} \\ d_1u_{14}v_{11} + d_2u_{24}v_{21} \\ d_1u_{14}v_{12} + d_2u_{24}v_{22} \end{bmatrix}$$

Appendix. Partial trace and the reduced density operator.

Consider a generic, pure three qubit state $|\psi\rangle = a|000\rangle + b|001\rangle + c|010\rangle + d|011\rangle + e|100\rangle + f|101\rangle + g|110\rangle + h|111\rangle$. The density operator is

$$\rho^{AB} =$$

$$\begin{aligned}
&a^2|000\rangle\langle 000| + ab|000\rangle\langle 001| + ac|000\rangle\langle 010| + ad|000\rangle\langle 011| + \\
&ae|000\rangle\langle 100| + af|000\rangle\langle 101| + ag|000\rangle\langle 110| + ah|000\rangle\langle 111| + \\
&ab\,|001\rangle\langle 000| + b^2|001\rangle\langle 001| + bc|001\rangle\langle 010| + bd|001\rangle\langle 011| + \\
&be|001\rangle\langle 100| + bf|001\rangle\langle 101| + bg|001\rangle\langle 110| + bh|001\rangle\langle 111| + \\
&ac\,|010\rangle\langle 000| + bc|010\rangle\langle 001| + c^2|010\rangle\langle 010| + cd|010\rangle\langle 011| + \\
&ce|010\rangle\langle 100| + cf|010\rangle\langle 101| + cg|010\rangle\langle 110| + ch|010\rangle\langle 111| + \\
&ad\,|011\rangle\langle 000| + bd|011\rangle\langle 001| + cd|011\rangle\langle 010| + d^2|011\rangle\langle 011| + \\
&de|011\rangle\langle 100| + df|011\rangle\langle 101| + dg|011\rangle\langle 110| + dh|011\rangle\langle 111| + \\
&ae\,|100\rangle\langle 000| + be|100\rangle\langle 001| + ce|100\rangle\langle 010| + de|100\rangle\langle 011| + \\
&e^2|100\rangle\langle 100| + ef|100\rangle\langle 101| + eg|100\rangle\langle 110| + eh|100\rangle\langle 111| + \\
&af\,|101\rangle\langle 000| + bf\,|101\rangle\langle 001| + cf|101\rangle\langle 010| + df|101\rangle\langle 011| + \\
&ef\,|101\rangle\langle 100| + f^2|101\rangle\langle 101| + fg|101\rangle\langle 110| + fh|101\rangle\langle 111| + \\
&ag\,|110\rangle\langle 000| + bg|110\rangle\langle 001| + cg\,|110\rangle\langle 010| + dg|110\rangle\langle 011| + \\
&eg|110\rangle\langle 100| + fg\,|110\rangle\langle 101| + g^2|110\rangle\langle 110| + gh|110\rangle\langle 111| + \\
&ah\,|111\rangle\langle 000| + bh|111\rangle\langle 001| + ch|111\rangle\langle 010| + dh\,|111\rangle\langle 011| + \\
&eh|111\rangle\langle 100| + fh|111\rangle\langle 101| + gh|111\rangle\langle 110| + h^2|111\rangle\langle 111|
\end{aligned}$$

Suppose system A refers to the first qubit and system B refers to qubits two and three. Then, reduced density operator ρ^A is retrieved by tracing out the last two qubits.

$$\begin{aligned}
\rho^A = (a^2+b^2+c^2+d^2)|0\rangle\langle 0| + (ae+bf+cg+dh)|0\rangle\langle 1| + \\
(ae+bf+cg+dh)|1\rangle\langle 0| + \left(e^2+f^2+g^2+h^2\right)|1\rangle\langle 1|
\end{aligned}$$

Further, reduced density operator ρ^B involves tracing out the first qubit.

$$\rho^B =$$

$$\begin{aligned}
&(a^2+e^2)|00\rangle\langle 00| + (ab+ef)|00\rangle\langle 01| + (ac+eg)|00\rangle\langle 10| + (ad+eh)|00\rangle\langle 11| + \\
&(ab+ef)|01\rangle\langle 00| + (b^2+f^2)|01\rangle\langle 01| + (bc+fg)|01\rangle\langle 10| + (bd+fh)|01\rangle\langle 11| + \\
&(ac+eg)|10\rangle\langle 00| + (bc+fg)|10\rangle\langle 01| + (c^2+g^2)|10\rangle\langle 10| + (cd+gh)|10\rangle\langle 11| +
\end{aligned}$$

$(ad + eh) |11\rangle \langle 00| + (bd + fh) |11\rangle \langle 01| + (cd + gh) |11\rangle \langle 10| + (d^2 + h^2) |11\rangle \langle 11|$

The foundation of singular value decomposition, $\alpha = udv^T$, is spectral decomposition of $\alpha\alpha^T = ud^2u^T$ or $\alpha^T\alpha = vd^2v^T$ where $\alpha = \begin{bmatrix} a & b & c & d \\ e & f & g & h \end{bmatrix}$ and only the first r columns of u and v are retained. Then, the connection between employing the partial trace and the spectral decomposition follows from

$$\alpha\alpha^T = \rho^A =$$
$$\begin{bmatrix} (a^2 + b^2 + c^2 + d^2) & (ae + bf + cg + dh) \\ (ae + bf + cg + dh) & (e^2 + f^2 + g^2 + h^2) \end{bmatrix}$$

and

$$\alpha^T\alpha = \rho^B =$$
$$\begin{bmatrix} (a^2 + e^2) & (ab + ef) & (ac + eg) & (ad + eh) \\ (ab + ef) & (b^2 + f^2) & (bc + fg) & (bd + fh) \\ (ac + eg) & (bc + fg) & (c^2 + g^2) & (cd + gh) \\ (ad + eh) & (bd + fh) & (cd + gh) & (d^2 + h^2) \end{bmatrix}$$