

## Singular Value Decomposition - quick review

- called SVD
- a basic tool from linear algebra.
- generalizes eigen-decomposition to non-square matrices.  
→ w/o proof:

Any matrix  $A \in \mathbb{C}^{m \times n}$  can be written in product form:

$$A_{m \times n} = U_{m \times m} \Sigma_{m \times n} V^T_{n \times n}$$

with:  $U, V$  unitary,

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & 0 & \end{bmatrix}_{m \times n} \quad \begin{array}{l} \in \sigma_1 > \sigma_2 > \dots > \sigma_r > 0 \\ \rightarrow \text{positive \& descending.} \end{array}$$

- example,

$$[A]_{m \times n} = [U]_{m \times m} \begin{bmatrix} \Sigma \\ \vdots \\ 0 & \ddots & 0 \end{bmatrix}_{m \times n} [V^T]_{n \times n}$$

rot<sup>r</sup> in output space      scaling along r axis.      rotation in input space

$$[A]_{m \times n} \begin{bmatrix} \sigma \\ \vdots \\ 0 \end{bmatrix}_{n \times 1} = [\ ]_{m \times 1} \quad \text{as matrix-vector mult.}$$

- $r$  is the rank of matrix  $A$  with  $r \leq \min(m, n)$  here.
- special case:

①  $r=1$  rank 1:  $A = \sigma u v^T = \sigma |u\rangle\langle v|$

- ② select  $k < r$  of the largest  $k$  singular values,  $\{\sigma_i\}_{i=1}^r$ :  
→ yields the closest in Euclidean norm rank  $k$

approximation of  $A \rightarrow$  used in PCA, recommender systems, photogrammetry, signal processing, ...

## Schmidt Decomposition

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- a useful canonical form in QIT.
- takes a (generally) messy superpositioned state into a simpler standard form by a coord transformation.
- it's the same state, just more compact.
- does this for a state in the tensor product of two Hilbert spaces:

### Theorem : Schmidt Decomposition.

Let  $H_A$  &  $H_B$  be two Hilbert spaces and  $|ψ\rangle \in H_A \otimes H_B$  a unit vector.

Then there exist ONB  $\{|i_A\rangle\} \subset H_A$  and  $\{|i_B\rangle\} \subset H_B$  and real numbers  $\{\lambda_i\} > 0 \in \sum_i \lambda_i^2 = 1$  such that:

$$|ψ\rangle = \sum_{i=1}^r \lambda_i |i_A\rangle \otimes |i_B\rangle.$$

- 
- it says that even though in an arbitrary ONB of the two Hilbert spaces a state vector can be expressed as a sum of up to  $d_A d_B$  product basis states, a unique ONB exists such that is the sum of only  $r$  product basis, with  $r \leq \min(d_A, d_B)$ .
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(3)

### Proof:

- in general you can always write some  $|\Psi\rangle \in H_A \otimes H_B$  as:

$$|\Psi\rangle = \sum_{j,k}^{d_A, d_B} c_{jk} |j\rangle_A \otimes |k\rangle_B$$

for any ONB  $\{|j\rangle_A\}$  in  $H_A$  and  $\{|k\rangle_B\}$  in  $H_B$ .

- we are going to rotate them to a new basis that reduces the sum from  $d_A d_B$  terms (in general) to  $r \leq \min(d_A, d_B)$ .

$\Rightarrow$  use SVD.

- put the coeff's  $c_{jk}$  into a matrix,  $C$ , such that

$$[C]_{jk} = c_{jk}$$

- take its SVD,

$$C = UDV^\dagger \in D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_r, 0, \dots, 0)$$

- then,

$$\begin{aligned} |\Psi\rangle &= \sum_{jk} [UDV^\dagger]_{jk} |j\rangle_A \otimes |k\rangle_B \\ &= \sum_{jk} \sum_i U_{ji} D_{ii} [V^\dagger]_{ik} |j\rangle_A \otimes |k\rangle_B \\ &= \sum_{jk} \sum_i U_{ji} D_{ii} V_{ki}^* |j\rangle_A \otimes |k\rangle_B \\ &= \sum_i \lambda_i \left( \sum_j U_{ji} |j\rangle_A \right) \otimes \left( \sum_k V_{ki}^* |k\rangle_B \right) \end{aligned}$$

$$|\Psi\rangle = \sum_i \lambda_i |i_A\rangle \otimes |i_B\rangle$$

where:  $|i_A\rangle \equiv \sum_j U_{ji} |j\rangle_A$

$$|i_B\rangle \equiv \sum_k V_{ki}^* |k\rangle_B$$

## Example:

Suppose we want to build rank 1 decomposition for a qubit  $\lambda^{\text{pair}}$   $|\Psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ .

since there are only two singular values,

$$\lambda_1 = 1, \quad \lambda_2 = 0.$$

$$\therefore D = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

take  $U$  &  $V$  to be real orthogonal:

$$U = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \quad V = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}$$

the coefficient matrix is:

$$C = UDV^\dagger$$

$$= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{where } a = \cos\theta \cos\phi, \quad b = \cos\theta \sin\phi \\ c = \sin\theta \cos\phi, \quad d = \sin\theta \sin\phi$$

we have the new basis:

$$|2'_A\rangle = \sum_j U_{j1} |j\rangle_A \Rightarrow |0'_A\rangle = \cos\theta |0\rangle_A + \sin\theta |1\rangle_A \\ |0'_B\rangle = \cos\phi |0\rangle_B + \sin\phi |1\rangle_B.$$

$|\Psi\rangle$  in the new basis is:

$$|\Psi\rangle = 1 \cdot |0'_A\rangle \otimes |0'_B\rangle$$

← a pure state as expected  
with  $r=1$

note the  $|1'_A\rangle \otimes |1'_B\rangle$  is multiplied by  $\lambda_2 = 0$ .

$$\text{check: expand } |0'_A\rangle \otimes |0'_B\rangle = (c_0 |0\rangle_A + s_0 |1\rangle_A) \otimes (c_\phi |0\rangle_B + s_\phi |1\rangle_B) \\ = \underbrace{c_0 c_\phi}_{a} |00\rangle + \underbrace{c_0 s_\phi}_{b} |01\rangle + \underbrace{s_0 c_\phi}_{c} |10\rangle + \underbrace{s_0 s_\phi}_{d} |11\rangle$$

→ see  $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$  entries above. ✓

## Question?

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Where did the degrees of freedom go?

- a general ket  $| \Psi \rangle$  in  $H_A \otimes H_B$  has the form

$$| \Psi \rangle = \sum_{j,k=1}^{d_A \cdot d_B} c_{jk} | j \rangle_A \otimes | k \rangle_B$$

for an arbitrary ONB  $\{ | j \rangle_A \}$  and  $\{ | k \rangle_B \}$  on  $H_A$  &  $H_B$ .

- this can have up to  $d_A \cdot d_B$  non-zero coefficients (dof)
- but under a new ONB,  $\{ | i_A \rangle \}, \{ | i_B \rangle \}$ , we can write it:

$$| \Psi \rangle = \sum_{i=1}^r \lambda_i | i_A \rangle \otimes | i_B \rangle$$

$\Rightarrow$  where  $r \leq \min(d_A, d_B)$ .

- how did we go from  $d_A \cdot d_B$  dof to  $\min(d_A, d_B)$  without losing something?

$\Rightarrow$  they're in the special basis vectors that make it work!

## Quick Explanation:

- original  $c_{jk}$  coefficients are in the  $C_{d_A \times d_B}$  matrix  
 $\Rightarrow 2d_A \cdot d_B - 1$  dof. (subtract 1 for  $\sum_{jk} |c_{jk}|^2 = 1$  norm. constraint  
↑ "complex")
- we have the SVD:

$$\left[ \begin{array}{c} \\ \end{array} \right]_{d_A \times d_B} = \left[ \begin{array}{c|c} \vdots & \vdots \\ \hline U & V \end{array} \right]_{d_A \times d_B} \left[ \begin{array}{c|c} \ddots & 0 \\ \hline 0 & 0 \end{array} \right]_{d_A \times d_B} \left[ \begin{array}{c|c} \vdots & \vdots \\ \hline 0 & 0 \end{array} \right]_{d_B \times d_B} V^T$$

- note: Only the first  $r$  columns of  $U$  &  $V$  actually count in the matrix mult:

$\Rightarrow$  the first  $r$  singular values keep them.  
- the rest of the 0-diagonal elts nullify the rest of the columns.

Picture:

$$\begin{bmatrix} & \\ & \end{bmatrix}_{d_A \times d_B} = \begin{bmatrix} & \\ & \end{bmatrix}_{r \times r}^T \begin{bmatrix} & \\ & \end{bmatrix}_{r \times r} \begin{bmatrix} \ddots & & \\ & 0 & \\ & & 0 \end{bmatrix} \begin{bmatrix} & \\ & \end{bmatrix}_{r \times r}^T \begin{bmatrix} & \\ & \end{bmatrix}_{d_B \times d_B}^T.$$

U       $\Sigma$       V

Count of dof:

- singular values:  $r$  (real)
- U matrix:  $2rd_A$  (complex)
- V matrix:  $-r^2$  (orthonormality/inner product constraint)
- basis vectors:  $2rd_B$
- phases btwn A-B basis vectors:  $-r$
- global phase:  $\frac{-1}{2(d_A+d_B)r - 2r^2 - 1}$

- say  $d_A$  is the smallest dim  $\Leftrightarrow r=d_A$  to maximize dof:

$$\Rightarrow 2(d_A + d_B)d_A - 2d_A^2 - 1$$

$$= 2d_A^2 + 2d_Ad_B - 2d_A^2 - 1$$

$$= 2d_Ad_B - 1$$

$\Rightarrow$  equals dof of C matrix!

# ENTANGLEMENT (Finally!)

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- consider a single state  $|\Psi\rangle_{AB}$  in  $H_A \otimes H_B$ .
- it is a product state if we can write it in the form  

$$|\Psi\rangle_{AB} = |U\rangle_A \otimes |V\rangle_B.$$

$\Rightarrow$  it is determined by a single vector in  $H_A$  and a single vector in  $H_B$ , separately!
- this is a special (trivial) case of a Schmidt decomposition,

$$|\Psi\rangle = \sum_{i=1}^r \sigma_i |i_A\rangle \otimes |i_B\rangle$$

where:  $r=1$

$$\sigma_1 = 1$$

$$|i_A\rangle = |U\rangle_A, |i_B\rangle = |V\rangle_B.$$

- suppose we have some other  $|\phi\rangle \in H_A \otimes H_B$  and do a S.D.

$$|\phi\rangle = \sum_{i=1}^r \sigma_i |i_A\rangle \otimes |i_B\rangle \quad \text{where } r > 1.$$

$\rightarrow$  this decomp<sup>n</sup> is unique and  $r$  is the smallest possible  
 $\Rightarrow$  if  $r > 1$  we say the state is entangled.

That is, if we can't write a state vector as a single tensor product,  $|\Psi\rangle_{AB} = |U\rangle_A \otimes |V\rangle_B$ , and must include more as a sum, e.g.  $|\Psi\rangle \propto |U_1\rangle_A \otimes |V_1\rangle_B + |U_2\rangle_A \otimes |V_2\rangle_B + \dots$ , then it is entangled.

- so by def<sup>n</sup>: "Entangled"  $\Leftrightarrow$  Schmidt rank  $> 1$ .

The intuition is that if we can't describe the joint state in  $H_A \otimes H_B$  by two separate independent substate vectors in  $H_A$  &  $H_B$ , they are entangled in their behaviour.

alone

"Not entangled"  $\Leftrightarrow$  "Separable/Factored"  $\Leftrightarrow$  Schmidt  $r=1$

Here is where it gets confusing:

You are dealing with 3 different binary conditions-

- ① Compositeness: i) 1 qubit, ii) 2 qubits
  - ② Purity: i) single state vector,  $| \Psi \rangle$  (pure)  
ii) ensemble of state vectors,  $\{ | \Psi_i \rangle, p_i \}$  (mixed)
  - ③ Entanglement: i) Separable (can be factored)  
ii) entangled.
- 

Start with:

### ① Single Qubit/Quantum System:

- so a single Hilbert state space,  $H_A$ .

NOT:  $H_A \otimes H_B$ .

$\therefore$  entanglement (i.e., being separable or entangled) does not enter the picture.

Only two cases to consider then for Purity: <sup>i)</sup> pure, or <sup>ii)</sup> mixed

#### ii) Purity = pure:

- a state is a single vector,  $| \Psi \rangle \in H_A$

- density matrix  $\rho = | \Psi \rangle \langle \Psi |_A$

Test:

- i) rank 1
- ii) single non-zero eigenvalue
- iii)  $\text{Tr} \rho^2 = 1$

} equivalent.

#### ii) Purity = mixed:

- $| \Psi \rangle$  is drawn from an ensemble or distribution,  $\{ | \Psi_i \rangle, p_i \}$

- a density matrix  $\rho = \sum_{i=1}^{n+1} p_i | \Psi_i \rangle \langle \Psi_i |$

Test:

- i) rank  $> 1$
- ii) more than one non-zero eigenvalue
- iii)  $\text{Tr} \rho^2 < 1$ .

Now consider:

## ② Bipartite (composite) 2 Qubit System:

- a Hilbert space given by  $H_A \otimes H_B$ .

→ entanglement is possible.

### A Purity = pure:

- system described by a single state vector:  $|\Psi\rangle_{AB}$

- density matrix  $\rho_{AB} = |\Psi\rangle_{AB} \langle \Psi|_{AB}$

- again test for purity is:

- $\rho$  is:
  - rank 1
  - one eigenvalue
  - $\text{tr } \rho^2 = 1$

Now test for entanglement: Two cases:

### i) Separable

→ we can factorize the state into a single

tensor product:  $|\Psi\rangle_{AB} = |\phi_A\rangle \otimes |\phi_B\rangle$

for some  $|\phi_A\rangle \in H_A$ ,  $|\phi_B\rangle \in H_B$ .

Test: Schmidt rank  $r=1$ .

- quick test for two level bipartite system:

- general  $|\Psi\rangle_{AB} = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$ .

- coeff. matrix  $C = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \neq 0$ .

→ iff a singular value/eigenvalue is 0 then  
 $C$  is singular and  $\det C = 0$ .

⇒ then  $r=1$  & vector is separable.

$\therefore ab - bc = 0 \iff$  not entangled  
 $\neq 0 \iff$  entangled.

ii) Entangled: Schmidt rank  $r>1$  (cannot cleanly factor state)

Example:

$$\textcircled{1} \quad |\Psi\rangle_{AB} = |00\rangle + |01\rangle$$

$$\therefore C = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \neq 0$$

$$\det C = 1 \cdot 0 - 1 \cdot 0 = 0.$$

$\therefore C$  is rank 1 a separable (not entangled).

Why?: Writk:

$$\begin{aligned} |\Psi\rangle_{AB} &= |00\rangle + |01\rangle \\ &= |0\rangle_A \otimes |0\rangle_B + |0\rangle_A \otimes |1\rangle_B \\ &= |0\rangle_A \otimes \left( |0\rangle_B + |1\rangle_B \right) \\ &\quad \delta \quad \underbrace{\quad}_{H_A} \quad \underbrace{\quad}_{\in H_B} \end{aligned}$$

$$\textcircled{2} \quad |\Psi\rangle_{AB} = (|00\rangle + |11\rangle) / \sqrt{2}.$$

$$\Rightarrow C \propto \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}.$$

$$\det C = \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} - 0 \cdot 0$$

$$= \frac{1}{2} \neq 0.$$

$\therefore C$  is Schmidt rank 2 and is entangled.

What about mixed bipartite systems?

$\Rightarrow$  much more complicated situation

- need to define what "factoring" a state/density matrix even means

$\Rightarrow$  generally, an NP-hard problem!

# Categories of Compositeness, Purity, and Entanglement

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Table 1: Quantum system conditions — Compositeness / Purity / Entanglement

Condition	Type
Compositeness	<b>Single Qubit: A</b> $ \psi\rangle_A =  0\rangle_A$ $ \psi\rangle_A =  0\rangle_A +  1\rangle_A$ <b>Two Qubits: AB (Composite, Bipartite)</b> $ \psi\rangle_{AB} =  01\rangle_{AB}$ $ \psi\rangle_{AB} =  00\rangle_{AB} +  01\rangle_{AB}$
Purity	<b>Single State Vector (Pure)</b> $ \psi\rangle_A,  \psi\rangle_{AB}$ $\rho_A =  \psi\rangle_A \langle\psi _A$ $\rho_{AB} =  \psi\rangle_{AB} \langle\psi _{AB}$ <b>Ensemble of SV's (Mixed, Mixture)</b> $\{ \psi_i\rangle, p_i\}$ $\rho = \sum_i p_i  \psi_i\rangle \langle\psi_i $
Entanglement	<b>Separable (Factored)</b> $ \psi\rangle_{AB} =  1\rangle_A \otimes  0\rangle_B$ $ \psi\rangle_{AB} =  0\rangle_A \otimes ( 0\rangle_B +  1\rangle_B)$ <b>Entangled</b> $ \psi\rangle_{AB} =  0\rangle_A \otimes  0\rangle_B +  1\rangle_A \otimes  1\rangle_B$

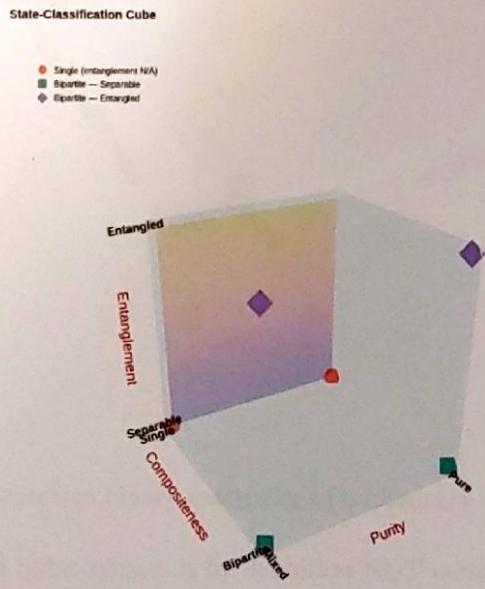


Figure 1: The three descriptive binary categories of a quantum system: Compositeness, Purity and Entanglement.  
**Note:** A single isolated qubit system is by definition NOT entangled with another. So two of the top corners of the cube, (Single, Entangled, Pure/Mixed), are not valid and left empty.

State-Classification Cube

- Single (entanglement NOT)
- Bipartite — Separable
- ◆ Bipartite — Entangled

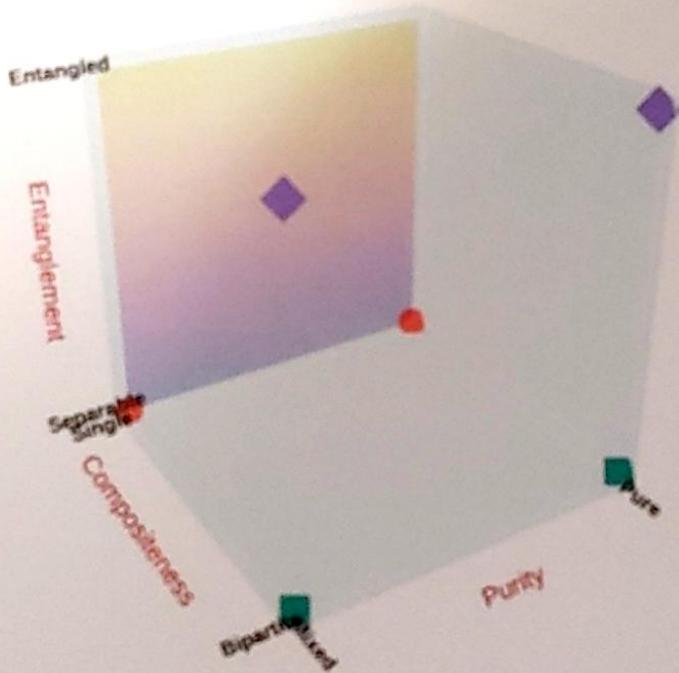


Figure 2: The three descriptive binary categories of a quantum system: Compositeness, Purity and Entanglement.

**Note:** A single isolated qubit system is by definition NOT entangled with another. So two of the top corners of the cube, (Single, Entangled, Pure/Mixed), are not valid and left empty.