Gram-Schmidt orthonormalization process

Let $\{|x_1\rangle, \ldots, |x_m\rangle\}$ be linearly independent.
We can use the following Gram-Schmidt process to construct an orthonormal set $\{|e_1\rangle, \ldots, |e_m\rangle\}$ such that

$$\text{span}\{|x_1\rangle, \ldots, |x_\ell\rangle\} = \text{span}\{|e_1\rangle, \ldots, |e_\ell\rangle\},$$

for all $\ell = 1, \ldots, m$.

Set $|e_1\rangle = |x_1\rangle / \| |x_1\rangle \|$.

For $k > 1$, set $|f_k\rangle / \| |f_k\rangle \|$, where

$$|f_k\rangle = |x_k\rangle - a_1|e_1\rangle - \cdots - a_{k-1}|e_{k-1}\rangle$$

with $a_j = \langle e_j | x_k \rangle$.

We can further extend the set to an o.n. basis

Let $\{|y_1\rangle, \ldots, |y_n\rangle\} \subseteq \mathbb{C}^n$ be a basis.

Find linearly independent columns of the matrix

$$[|e_1\rangle \cdots |e_m\rangle |y_1\rangle \cdots |y_n\rangle]$$

including the first m columns.

Then apply Gram-Schmidt process.

Example Apply Gram-Schmidt to $\{|x_1\rangle, |x_2\rangle\}$ with

$$|x_1\rangle = \begin{pmatrix} 1 \\ 1 \\ i \end{pmatrix}, \; |x_2\rangle = \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}.$$

Then extend the resulting set to an orthnormal basis.

Basics of Matrices

- Mixed quantum states are represented by density matrices, i.e., positive semi-definite matrices with trace 1.
- Observable / measurement operators correspond to Hermitian matrices.
- Quantum operations corresponds to unitary matrices.
- So, we need basic knowledge of matrices (relevant to quantum mechanics).

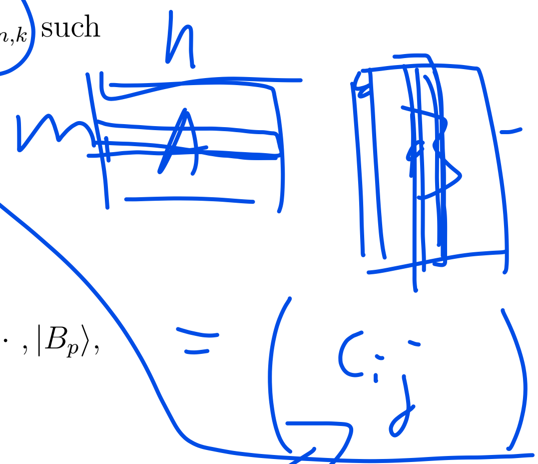
Let $\mathbf{M}_{m,n}$ be the set (vector space/algebra) of $m \times n$ complex matrices. If $m = n$, we let $\mathbf{M}_n = \mathbf{M}_{m,n}$.

$M_{2,3}$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix}$$

- The set $\mathbf{M}_{m,n}$ is a vector space under addition and scalar multiplication.
- We can multiply $A = (a_{ij}) \in \mathbf{M}_{m,n}$ and $B = (b_{rs}) \in \mathbf{M}_{n,k}$ such that $C = AB = (c_{pq}) \in \mathbf{M}_{m,k}$ with

$$c_{pq} = (a_{p1}, \dots, a_{pn}) \begin{pmatrix} b_{1q} \\ \vdots \\ b_{nq} \end{pmatrix} = \sum_{\ell=1}^{n} a_{p\ell} b_{\ell q}.$$



- If A has rows $\langle A_1|, \dots, \langle A_m|$ and B has columns $|B_1\rangle, \cdots, |B_p\rangle$, then

$$AB = [A|B_1\rangle \cdots A|B_p\rangle] = \begin{pmatrix} \langle A_1|B \\ \vdots \\ \langle A_m|B \end{pmatrix}$$

$m \times n \quad n \times p$

$$A\,[\,|B_1\rangle \cdots |B_p\rangle\,] = [\,A|B_1\rangle \quad A|B_p\rangle\,]$$

$$\begin{pmatrix} \langle A_1| \\ \langle A_2| \\ \\ \langle A_m| \end{pmatrix} B = \begin{bmatrix} \langle A_1|B \\ \vdots \\ \langle A_m|B \end{bmatrix}$$

Block matrix multiplication.

- If $A = (A_{ij}), B = (B_{rs})$ such that $A_{p\ell}B_{\ell q}$ is defined. That is, the number of columns of $A_{p\ell}$ equals the number of rows of $B_{\ell q}$.

- If $D = \operatorname{diag}(d_1, \ldots, d_n)$, A has columns $|x_1\rangle, \ldots, |x_n\rangle$, and B has rows $\langle y_1|, \ldots, \langle y_n|$, then

$$AD = [d_1|x_1\rangle \cdots d_n|x_n\rangle], \quad DB = \begin{pmatrix} d_1\langle y_1| \\ \vdots \\ d_n\langle y_n| \end{pmatrix},$$

$$AB = \sum_{j=1}^{n} |x_j\rangle\langle y_j|, \quad ADB = \sum_{j=1}^{n} d_j|x_j\rangle\langle y_j|.$$

- If $A \in \mathbf{M}_{m,n}, B \in \mathbf{M}_{n,k}, D = D_1 \oplus \mathbf{0}_{n-\ell}$, then

$$ADB = A\begin{pmatrix} D_1 & 0 \\ 0 & 0 \end{pmatrix}B = A_1D_1B_1,$$

where A_1 is formed by the first ℓ columns of A and B_1 is formed by the first ℓ rows of B.

Eigenvalues and eigenvectors

$\boxed{A|x\rangle} = \lambda|x\rangle$

- Let $A \in \mathbf{M}_n$. We would like to find nonzero $|x\rangle \in \mathbb{C}^n$ such that $A|x\rangle = \lambda|x\rangle$.

  Then λ is an eigenvalue associated with the eigenvector $|x\rangle$.

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- If one can find n linearly independent set $\{|x_1\rangle, \ldots, |x_n\rangle\}$ of eigenvectors, then we can let $S = [|x_1\rangle \cdots |x_n\rangle]$ such that

  $\rightarrow$ basis $\mathbb{C}^n$

  $$\longleftrightarrow \boxed{AS = [\lambda_1|x_1\rangle \cdots \lambda_n|x_n\rangle] = SD} \quad \lambda_1 \cdots \lambda_n$$

  with $D = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$. So, $\boxed{S^{-1}AS = D.}$

  $A = SDS^{-1}$

- To compute the eigenvalues and eigenvectors of $A \in \mathbf{M}_n$, one solves the characteristic equation $\det(tI - A) = 0$, which is a polynomial equation.

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- For every t satisfying $\det(tI - A) = 0$, we solve for nonzero vectors $|x\rangle$ such that $A|x\rangle = t|x\rangle$.

- Important facts: $\operatorname{tr}A = \sum_{j=1}^n \lambda_j$, $\det(A) = \prod_{j=1}^n \lambda_n$.

- Not every matrix in $\mathbf{M}_n$ has n linearly independent eigenvectors.

$$S^{-1}\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} S = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = S\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} S^{-1} =$$

Special classes of matrices

- $A \in \mathbf{M}_n$ is Hermitian if $A = A^\dagger$. $= (A^*)^t$

  The (i,j) entry of A is the conjugate of the (j,i) entry of A.

- $A \in \mathbf{M}_n$ is unitary if $A^\dagger = A^{-1}$, i.e., $AA^\dagger = I_n$ or /and $A^\dagger A = I_n$.

  The columns of U form an orthonormal basis for $\mathbb{C}^n$.

- $A \in \mathbf{M}_n$ is positive semidefinite if $\langle x|A|x\rangle \geq 0$ for all $|x\rangle \in \mathbb{C}^n$.

  Equivalently, A is Hermitian with nonnegative eigenvalues.

- $A \in \mathbf{M}_n$ is normal if $AA^\dagger = A^\dagger A$.

$$\begin{bmatrix} 1 & 1+i \\ 1-i & 2 \end{bmatrix}$$

$$[a_{ij}] \qquad \langle x|A|x\rangle \geq 0 \qquad x^* A x$$

$$\begin{bmatrix} \langle A_1| \\ \vdots \\ \langle A_n| \end{bmatrix} \underbrace{\begin{bmatrix} |A_1\rangle & \cdots & |A_n\rangle \end{bmatrix}}_{} = \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \neq \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

Spectral decomposition of a normal matrix

Theorem A matrix $A \in \mathbf{M}_n$ is normal if and only if there is a unitary $U = [|u_1\rangle \cdots |u_n\rangle]$ and unitary $D = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ such that

$$A = UDU^\dagger = \sum_{j=1}^{n} \lambda_j |u_j\rangle\langle u_j|.$$

That is A has an orthonormal set of eigenvectors $\{|u_1\rangle, \ldots, |u_n\rangle\}$ for the eigenvalues $\lambda_1, \ldots, \lambda_n$ so that

$$\boxed{A[|u_1\rangle \cdots |u_n\rangle] = [|u_1\rangle \cdots |u_n\rangle]D.}$$

So, $U^\dagger AU = D$.

Corollary Let $A \in \mathbf{M}_n$.

- Then A is Hermitian if and only if A is normal with real eigenvalues.
- Then A is unitary if and only if A is normal with eigenvalues on of modulus 1.
- Then A is positive semidefinite if and only if A is normal (Hermitian) with nonnegative eigenvalues.

$A = A^\dagger = A^2$

$AA^\dagger = A^\dagger A$

$AA^\dagger = I_n$

$A^\dagger A = I_n$

$\begin{bmatrix} 2 & 1 \\ 0 & 1 \end{bmatrix} = S \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} S^{-1}$

$U^\dagger A U = \begin{pmatrix} a_1 & & 0 \\ & \ddots & \\ 0 & & a_n \end{pmatrix}$

$U^\dagger A U = \begin{pmatrix} e^{i\theta_1} & & 0 \\ & \ddots & \\ 0 & & e^{i\theta_n} \end{pmatrix}$

Spectral theorem of normal matrices

Theorem Suppose $A \in \mathbf{M}_n$ is normal in the form

$$A = UDU^\dagger = \sum_{j=1}^{n} \lambda_j |u_j\rangle\langle u_j|.$$

- If k is a positive integer, then $\boxed{A^k = \sum_{j=1}^n \lambda_j^k |u_j\rangle\langle u_j|}$.
- If A is invertible and k is a positive integer, then $A^{-k} = \sum_{j=1}^n \lambda_j^{-k} |u_j\rangle\langle u_j|$.
- If A has positive eigenvalues, then $A^r = \sum_{j=1}^n \lambda_j^r |u_j\rangle\langle u_j|$.
- If f is an analytic function, then $\boxed{f(A) = \sum_{j=1}^n f(\lambda_j) |u_j\rangle\langle u_j|}$.

For example: $e^A = \sum_{j=0}^\infty \frac{1}{n!} A^n = \sum_{j=1}^n e^{\lambda_j} |u_j\rangle\langle u_j|$.

If $H = H^\dagger = \sum_{j=1}^n h_j |u_j\rangle\langle u_j|$ with real eigenvalues $h_1, \ldots, h_n$, then

$$\boxed{e^{iH} = \sum_{j=1} e^{ih_j} |u_j\rangle\langle u_j|}$$

is unitary.

$$A^2 = \begin{bmatrix} |u_1\rangle & \cdots & |u_n\rangle \end{bmatrix} \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} \begin{bmatrix} \langle u_1| \\ \vdots \\ \langle u_n| \end{bmatrix}$$

$$= U \begin{pmatrix} \lambda_1^2 & & 0 \\ & \ddots & \\ & & \lambda_n \end{pmatrix} U^\dagger$$

$$= \lambda_1^2 [\ ][\ ] + \lambda_2^2 [\ ][\ ]$$

$$\sum (|u_j\rangle\langle u_j|)^2 = |u_j\rangle\langle u_j|$$

Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Remark If $A \in \mathbf{M}_2$ is Hermitian, then

$$A = (c_0, c_x, c_y, c_y) \cdot (\sigma_0, \sigma_x, \sigma_y, \sigma_z) = c_0 I_2 + c_x\sigma_x + c_y\sigma_z + c_z\sigma_z$$

with $c_0, c_x, c_y, c_z \in \mathbb{R}$.

Example In quantum computing, we often use e^{iaA}, where for a real unit vector $\mathbf{n} = (n_x, n_y, n_z)$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$

$$A = \mathbf{n} \cdot \sigma = (n_x, n_y, n_z) \cdot (\sigma_x, \sigma_y, \sigma_z) = \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix},$$

which has eigenvalues $1, -1$ and with eigenprojections

$$P_1 = \frac{1}{2}(I + A) = \begin{pmatrix} 1 + n_z & n_x - in_y \\ n_x + in_y & 1 - n_z \end{pmatrix}$$

and

$$P_2 = \frac{1}{2}(I - A) = \begin{pmatrix} 1 - n_z & -n_x + in_y \\ -n_x - in_y & 1 + n_z \end{pmatrix}.$$

Hence, $iaA = iaP_1 - iaP_2$ and

$$e^{iaA} = e^{ia}P_1 + e^{-ia}P_2 = \cos aI + i \sin aA.$$

Singular value decomposition

Theorem Let $A \in \mathbf{M}_{m,n}$ of rank k. There is an orthonormal set $\{|v_1\rangle, \ldots, |v_k\rangle\} \subseteq \mathbb{C}^n$ such that

$$A|v_j\rangle = s_j|u_j\rangle \qquad \text{for } j = 1, \ldots, k,$$

where $s_1 \geq \cdots \geq s_k > 0$, $\{|u_1\rangle, \ldots, |u_k\rangle\}$ is an orthonormal set in $\mathbb{C}^m$. Equivalently, there are unitary $U \in \mathbf{M}_m$ and $V \in \mathbf{M}_n$ so that

$$U^\dagger AV = \Sigma = \begin{pmatrix} D & 0_{m,n-k} \\ 0_{n-k,k} & 0_{m-k,n-k} \end{pmatrix}, \quad D = \operatorname{diag}(s_1, \ldots, s_k).$$

$AV = U\Sigma$

Consequently, $A = \sum_{j=1}^{k} s_j|u_j\rangle\langle v_j|$, where $s_1^2 \geq \cdots \geq s_k^2$ are the positive eigenvalues of $A^\dagger A$ and $AA^\dagger$.

Proof. Suppose $V^\dagger A^\dagger AV = \operatorname{diag}(s_1^2, \ldots, s_n^2)$ with $s_1 \geq \cdots \geq s_n \geq 0$. Then the columns of AV form an orthogonal set. Suppose the first k columns of AV are nonzero. Then $k \leq m$. Let $|u_i\rangle$ be the ith column of AV divided by s_i, and let $U \in \mathbf{M}_m$ with the first k columns equal to $|u_1\rangle, \ldots, |u_k\rangle$. Then $U^\dagger AV = \Sigma$. $\square$

$n \times n$

$A|x\rangle = \lambda|x\rangle$

$A|v_j\rangle = s_j|u_j\rangle$

$A = s_1|u_1\rangle\langle v_1| + \cdots + s_k|u_k\rangle\langle v_k|$

Example Let $A = \begin{pmatrix} 1 & 1 \\ 0 & 0 \\ i & i \end{pmatrix}$. Then $A^\dagger A = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$.

If $V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, then $V^\dagger A A V = \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix}$.

So, $\Sigma = \begin{pmatrix} 2 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$ and $AV = \begin{pmatrix} 2 & 0 \\ 0 & 0 \\ 2i & 0 \end{pmatrix}$.

We may take $U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ i & 0 & -i \end{pmatrix}$ to get $U^\dagger A V = \Sigma$.

Tensor products

Let $A = (A_{ij})$ and B be two rectangular matrices. Then their tensor product (Kronecker product) is the matrix

$$A \otimes B = (A_{ij}B).$$

$A = (A_{ij})$ $m \times n$

B is $p \times q$

This is very important in quantum mechanics.

If ρ_1, ρ_2 are quantum states of two quantum systems, then $\boxed{\rho_1 \otimes \rho_2}$ is their product state in the bipartite (combined) system.

$$A \otimes B \quad mp \begin{array}{c} nq \\ \begin{bmatrix} A_{11}B & A_{12}B & \\ & & \\ & & \end{bmatrix} \end{array}$$

Theorem *For matrices A, B, C, D of appropriate sizes, the following properties hold:*

(1) $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$.

(2) $A \otimes (B + C) = A \otimes B + A \otimes C$,

(3) $(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$,

(4) $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$.

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Proof. (1) Let $A \in \mathbf{M}_{m,n}$, $B \in \mathbf{M}_{r,s}$, $C \in \mathbf{M}_{n,p}$, and $D \in \mathbf{M}_{s,q}$. If $AC = (\gamma_{rs})$, then

$$\begin{aligned}(A \otimes B)(C \otimes D) &= (a_{ij}B)(c_{ij}D) = (\gamma_{rs}BD) \\ &= (\gamma_{rs}) \otimes (BD) = (AC) \otimes (BD).\end{aligned}$$

(2) $A \otimes (B + C) = (A_{ij}(B + C))$

$$= (A_{ij}B) + (A_{ij}C) = A \otimes B + A \otimes C.$$

(3) Let $\gamma_{rs} = \bar{A}_{sr}$. Then

$$(A \otimes B)^\dagger = (A_{ij}B)^\dagger = (\gamma_{rs}B^\dagger) = A^\dagger \otimes B^\dagger.$$

(4) Note that $(A^{-1} \otimes B^{-1})(A \otimes B) = I \otimes I$. $\square$

Corollary *For any matrices A, B, if*

$$R_1 A S_1 = T_1, R_2 B S_2 = T_2,$$

then $$(R_1 \otimes R_2)(A \otimes B)(S_1 \otimes S_2) = T_1 \otimes T_2.$$

Applications.

- *Let $A \in \mathbf{M}_m, B \in \mathbf{M}_n$. If*

  $$S_1^{-1} A S_1 = D_1, S_2^{-1} B S_2 = D_2,$$

  where D_1, D_2 are diagonal matrices, then

  $$(S_1 \otimes S_2)^{-1}(A \otimes B)(S_1 \otimes S_2) = D_1 \otimes D_2$$

  is a diagonal matrix.

  * If A, B are normal, we may assume that S_1, S_2 be unitary.*

  * If $A|u_i\rangle = \mu_i|u_i\rangle$ for $1 \le i \le m$, and $B|v_j\rangle = \nu_j|v_j\rangle$ $1 \le j \le n$,*

  then

  $$(A \otimes B)(|u_i v_j\rangle) = \mu_i \nu_j |u_i v_j\rangle,$$

  where $|u_i v_j\rangle = |u_i\rangle \otimes |v_j\rangle$.

- *If A, B are rectangular matrices with singular decomposition*

  $A = \sum_{i=1}^r a_i |u_i\rangle\langle v_i|$ *and* $B = \sum_{j=1}^s b_j |x_j\rangle\langle y_j|$,

  then

  $$A \otimes B = \sum_{r,s} a_i b_j |u_i x_j\rangle\langle v_i y_j|$$

  is the singular value decomposition of $A \otimes B$.

$A|x\rangle = \lambda|x\rangle$

$B|y\rangle = \mu|y\rangle$

$(A \otimes B)|x\rangle \otimes |y\rangle$

$= \lambda\mu|x\rangle \otimes |y\rangle$

$\lambda_1 \cdots \lambda_m$ A

$\mu_1 \cdots \mu_n$ B