LIQ/UI

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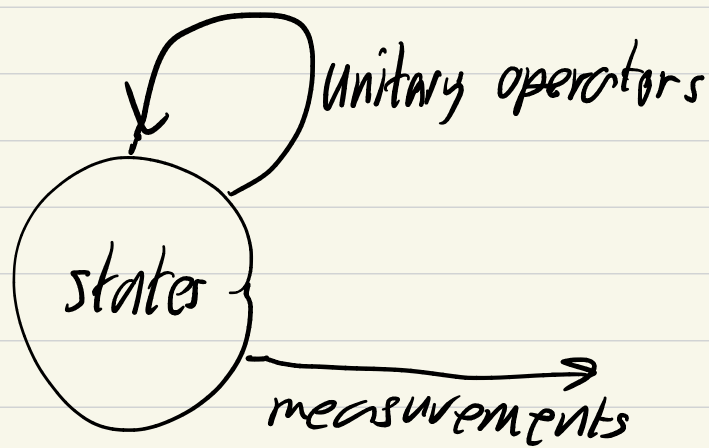
Quantum system:



Density Matrices

A complex square matrix M is **positive semidefinite** if

(a) $M = M^*$

(b) $u^* M u \geq 0, \ \forall u.$

If, in addition,

(c) $u^* M u = 0 \Rightarrow u = 0$, then M is **positive definite.**

We write $M \succeq N$ to denote that $M - N$ is psd.

If M is positive definite, we write $M \succ 0$.

Examples

(a) I

(b) gg^*

(c) If $M, N \succeq 0$, then $M+N \succeq 0$.

(d) any projection (why?)

If $A = [a_1, \dots, a_m]$ & $B = [b_1, \dots, b_m]$, both $n \times m$,

then

$$AB^* = a_1 b_1^* + \dots + a_m b_m^*$$

matrix multiplication using outer products

It follows that

(e) $AA^* \succeq 0$

A *density matrix* is a positive semidefinite matrix with trace one.

The simplest examples are the rank-one matrices zz^*, where $\|z\| \approx 1$. Note that zz^* represents projection onto the 1-dim. subspace spanned by z. If $a \in V(X)$, we call $e_a e_a^T$ a *vertex state*.

If $\|z\| = 1$, then zz^* is a *pure state*.

Lemma If M is positive definite, it is invertible.

Proof If $Mz = 0$, then $z^* M z = 0$ and so $z = 0$.

Hence $\ker(M) = \langle 0 \rangle$. $\square$

Show that if $M \succeq 0$ and $N \succ 0$, then

$M + N \succ 0$.

Lemma A convex combination of density matrices is a density matrix. $\square$

Lemma. Any psd matrix is a sum of positive semidefinite matrices of rank one. Any density matrix is a convex combination of pure states. $\square$

Theorem For a Hermitian matrix M, the following are equivalent:

(a) $M \succeq 0$, i.e. $u^* M u \geq 0$ for all u.

(b) $M = NN^*$ for some n

(c) all eigenvalues of M are non-negative.

(d) There are vectors $z_1, \dots, z_m$ and

$$M = z_1 z_1^* + \cdots + z_m z_m^*$$

$\mathrm{tr}(M^* N)$

(e) If $N \succeq 0$, then $\langle M, N \rangle \geq 0$.

We see that if $M \succeq 0$, then $\det(M) \geq 0$. Also

Lemma Any principal submatrix of a positive semidefinite is positive semidefinite. $\square$

2 × 2 density matrices

prove this is positive semidefinite.

$$\rho = \begin{pmatrix} \frac{1}{2}+a & b+ic \\ b-ic & \frac{1}{2}-a \end{pmatrix} \qquad \det(\rho) = \frac{1}{4} - a^2 - b^2 - c^2$$

If $M \succeq 0$, then its diagonal entries are non-negative; if the diagonal of M is zero, then $M = 0$.

Lemma If $M \succeq 0$, there is a unique psd matrix N s.t. $M = N^2$. $\square$

A quantum state is a density matrix.

Physicists will say that the state space of a quantum system is a separable Hilbert space (our state spaces will be finite) and a state is a unit vector. In fact the state is a 1-dim subspace of $\mathbb{C}^n$. The projection onto this subspace is a rank-one density matrix, that is, a pure state.

Operations on quantum states are given by unitary operators. If D is a state of a system & U is unitary, then applying U brings the system to a state UDU^{-1}.

If $D = zz^*$ (with $\|z\|=1$), then

$$UDU^{-1} = Uz\,z^*U^* = Uz\,(Uz)^*$$

$z \longmapsto Uz$

Bounds on cocliques

Let A be the adjacency matrix of a graph.

The A is real & symmetric, hence has a spectral decomp.

$$A = \theta_0 E_0 + \dots + \theta_d E_d$$

Our default assumption is that $\theta_0 \geq \dots \geq \theta_d$

Since $tr(A)=0$, we have $\sum_i \theta_i = 0$. So either

$\theta_0 > 0$ and $\theta_d < 0$, or $\theta_0 = \cdots = \theta_d = 0$ and $A = 0$. $\square$

Lemma If k is the maximum valency of a vertex of X, then $\theta_0 \leq k$.

Proof Assume $\underset{\sim}{z} \neq \underset{\sim}{0}$ and $A\underset{\sim}{z} = \theta_0 \underset{\sim}{z}$. Then

$$\theta_0 z_r = \sum_{i \sim r} z_i \qquad (*)$$

and, taking absolute values, we have

$$\theta_0 |z_r| \leq \sum |z_i|.$$

There are at most k terms in this sum. If r is chosen so $|z_r|$ is maximal, $\theta_0 \leq \sum_i \frac{|z_i|}{|z_r|} \leq k$. $\square$

Lemma A graph X is regular if and only if $\underline{1}$ is an eigenvector for A. $\square$

Lemma If X is k-regular then k is an eigenvalue of A with multiplicity equal to the number of components. $\square$

Lemma Let X be a graph on n vertices. The following are equivalent:

(a) X is connected and regular.

(b) J is a polynomial in A,

(c) $E_0 = \frac{1}{n} J$

A coclique in a graph X is a set S of vertices such that no two vertices in S are adjacent. (a.k.a. independent, stable) The maximum size of a coclique in X is denoted by $\alpha(X)$.

Hoffman, Delsarte

Theorem If X is k-regular with least eigenvalue τ, then

$$\alpha(X) \leq \frac{v}{1 - \frac{k}{\tau}}$$

If x is the characteristic vector of a coclique of size $v/(1-\frac{k}{\tau})$, then $x_S - \frac{|S|}{v}\mathbb{1}$ is an eigenvector for X with eigenvalue τ.

Proof. Assume $S \subseteq V(X)$ with characteristic vector x. Then $x^T A x$ is the number of pairs (u,v) in $S \times S$ with $u \sim v$. Hence S is a coclique if & only if $x^T A x = 0$.

Next, set

$$B = A - \frac{k-\tau}{v} - \tau I$$

Then $B \succcurlyeq 0$ and so $x^T B x \geqslant 0$. Now

$$0 \leq x^T B x = x^T A x - \frac{k-\tau}{v} x^T J x - \tau x^T x$$

$$= 0 - \frac{(k-\tau)|S|^2}{v} - \tau |S|$$

and therefore $|S| \leq \dfrac{v}{1-k\tau}$.

The rest is left as an exercise. $\square$