Density matrices with and without symmetry

Mary Beth Ruskai
marybeth.ruskai@tufts.edu

Tufts University

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Quantum marginal problem

ρ denotes density matrix (density operator) in $\mathcal{B}(\mathcal{H})$

$\text{Tr}\,\rho = 1$ and $\rho \geq 0$ pos semi-def

Basic Hilbert space $\mathcal{H}$ and consider $\mathcal{H} \otimes \mathcal{H} \otimes \ldots \mathcal{H} = \mathcal{H}^{\otimes m}$

e.g., qubit $\mathcal{H} = \mathbf{C}_2$ spin-$\frac{1}{2}$ particle

∞-dim $\rho(x; y)$ or $\rho(x_1, x_2, \ldots x_m; y_1, y_2, \ldots y_m)$ is integral kernel

Quant marginal asks: given $\rho_A, \rho_{AB}, \ldots$ does

$\exists\ \rho_{ABC\ldots}$ such that $\text{Tr}_{BC}\,\rho_{ABC} = \rho_A$ etc?

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Given ρ_A, ρ_{BC} does $\exists$ pure ρ_{ABC}

Answer: $\Leftrightarrow$ ρ_A and ρ_{BC} have same non-zero evals.

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for class prob dist $p(x, y)$, $p(x) = \int p(x, y) dy$ etc. called marginal

Different types of symmetry

regard N-rep as special case since perm symmetry $\Rightarrow \rho_A = \rho_B$ etc.

Assume finite dims $\mathcal{H} = \mathbf{C}^n$ or span$\{f_1, f_2, \ldots f_n\}$ fixed O.N. $\in \mathcal{H}$.

$d_{j_1 j_2 \ldots j_m, k_1 k_2 \ldots k_m}$ matrix els, $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ in prod basis for $\mathcal{H}^{\otimes m}$

Let $\mathcal{P}(j_1\, j_2 \ldots j_m)$ denotes perm of indices, e.g., $j_2\, j_1\, j_3 \ldots j_m$

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Fermions: want anti-symmetric if either set of indices permuted

$$d_{\mathcal{P}(j_1 j_2 \ldots j_m), k_1 k_2 \ldots k_m} = d_{j_1 j_2 \ldots j_m, \mathcal{P}(k_1 k_2 \ldots k_m)} = (-)^{\mathcal{P}} d_{j_1 j_2 \ldots j_m, k_1 k_2 \ldots k_m}$$

Bosons: want symmetric if either set of indices permuted

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N-representability problem:

Given m-particle D.M. ρ of right perm symmetry, when does $\exists$

- anti-symmetric N-particle pure state ψ such that

  $$\mathrm{Tr}_{m+1,\ldots N}\, |\psi\rangle\langle\psi| = \rho \ ??$$

- N-particle fermionic mixed state $\rho_{1,2\ldots N} = \sum_k a_k |\psi_k\rangle\langle\psi_k|$ s.t

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Most interest is $m = 2$; mixed $m = 1$ solved by Coleman ($\approx$ 1963)

pure state $m = 1$ solved by Klyachko (2005) for any symmetry

diFinettit theorems – exchangeable systems

Simultaneous perms $d_{\mathcal{P}(j_1 j_2 \ldots j_m),\mathcal{P}(k_1 k_2 \ldots k_m)} = d_{j_1 j_2 \ldots j_m, k_1 k_2 \ldots k_m}$

ρ could be convex comb. of boson and fermion states

or even more general

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perm symmetry plays two roles in N-rep of two particle RDM

a) Pauli principle itself

b) can use reduced Ham for 2-matrix

with simul or "exchangeable" perm symmetry, still have (b)

$$H_N = \sum_{k=1}^{N} T_k + \sum_{j<k} V_{jk} \qquad \widehat{H}_N = N T_1 + \binom{N}{2} V_{12}$$

$$\langle \Psi, H_N \Psi \rangle = \mathrm{Tr}\, H_N \, \rho_{1,2\ldots N} = \mathrm{Tr}\, \widehat{H}_N \, \rho_{12}$$

Where is perm symmetry in quantum Info

No perm symmetry because spatial wave function suppressed

real electron $\mathcal{H} = L_2(\mathbf{R}_3) \otimes \mathbf{C}_2$

quant info – consider pure state arbitrary vector in $\mathbf{C}_2^{\otimes n}$ or $\mathbf{C}_d^{\otimes n}$

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$$\psi(x_1, x_2) = f_A(\mathbf{r}_1) \uparrow \otimes f_B(\mathbf{r}_2) \downarrow - f_B(\mathbf{r}_1) \downarrow \otimes f_A(\mathbf{r}_2) \uparrow$$

with f_A and f_B supported in Alice and Bob's labs resp.

product corresponds to Slater det for full wave functions

Alice and Bob share entangled state $|01\rangle + |10\rangle$

symmetric not anti-sym – can still be done with electrons

$$\begin{aligned}
\psi(x_1, x_2) &= f_A(\mathbf{r}_1) \uparrow \otimes f_B(\mathbf{r}_2) \downarrow - f_B(\mathbf{r}_1) \downarrow \otimes f_A(\mathbf{r}_2) \uparrow \\
&\quad + f_A(\mathbf{r}_1) \downarrow \otimes f_B(\mathbf{r}_2) \uparrow - f_B(\mathbf{r}_1) \uparrow \otimes f_A(\mathbf{r}_2) \downarrow \\
&= \big(|01\rangle + |10\rangle\big) \big[f_A(\mathbf{r}_1) f_B(\mathbf{r}_2) - f_B(\mathbf{r}_1) f_A(\mathbf{r}_2) \big]
\end{aligned}$$

actually superposition of Slater dets.

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actually superposition of Slater dets.

Have $\psi = ($ spin $) \times [$ spatial $]$

General case – space and spin transform as dual Young tableux

Aside: polar cones

Thm: If ρ_{12} is not N-rep, then $\exists\ H_N \geq 0$ s.t. $\operatorname{Tr} \widehat{H}_N \, \rho_{12} < 0$.

Thm: If ρ_{12} is entangled, then $\exists$ positivity preserving map $\Gamma : \mathcal{B}(\mathcal{H}) \mapsto \mathcal{B}(\mathcal{H})$ such that $(I \otimes \Gamma)(\rho_{12}) < 0$.

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set of (mixed) N-rep D.M. is convex subset of all m-particle D.M.

set of separable states is convex subset of all states

separable means not entangled or convex comb of prod

entanglement witness Γ detects not separable

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Both results special cases of well known convex duality results

N-rep of 1-matrix as constrained version of Weyl's problem

Thm: (Ando-Coleman)The 1-matrix γ is pure N-rep with preimage

$\Leftrightarrow \qquad \gamma = \lambda_1 |\phi_1\rangle\langle\phi_1| + \lambda_1 \gamma_1 + (1 - \lambda_1)\gamma_2$

with γ_1 $N\!-\!1$-rep with pre-image Φ_1: γ_2 N-rep with pre-image Φ_2

and strong orthog $\langle \phi_1, \Phi_1 \rangle_1 = \langle \phi_1, \Phi_2 \rangle_1 = \langle \Phi_1, \Phi_2 \rangle_{2,3\ldots N} = 0$

pre-image $\quad |\Psi\rangle = \sqrt{\lambda_k}\, \mathcal{A}\, |\phi_1\rangle \otimes |\Phi_1\rangle + \sqrt{1 - \lambda_1}\, |\Phi_2\rangle$

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Consider special case $R = N + 3$ even, and

assume γ_2 has e-vec g_1 strong. orthog. to Φ_1 with eval 1

not wlog, but simplifies notation

$$\gamma - \lambda_1|\phi_1\rangle\langle\phi_1| - (1-\lambda_1)|g_1\rangle\langle g_1| = \lambda_1\gamma_1 + (1-\lambda_1)\widetilde{\gamma}_2.$$

Write
$$|\Phi_1\rangle = \sum_{2\leq k_1<k_2<\ldots k_{N-1}} x_{k_1 k_2 \ldots k_{N-1}} [g_{k_1}, g_{k_2}, \ldots g_{k_{N-1}}]$$
$$|\Phi_2\rangle = \sum_{2\leq k_1<k_{k_2}<\ldots k_{k_{N-1}}} y_{k_1 k_{k_2} \ldots k_{k_{N-1}}} [g_1, g_{k_1} g_{k_2}, \ldots g_{k_{N-1}}]$$

For anti-sym tensors let $x_{j,K} \equiv x_{j,k_2,k_3 \ldots k_M}$

$$XZ^\dagger = \sum_{k_2,k_3 \ldots k_M} x_{i,k_2,\ldots k_M} \, \overline{z}_{j,k_2,\ldots k_M}$$

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Rewrite above $\gamma - \lambda_1|\phi_1\rangle\langle\phi_1| - (1-\lambda_1)|g_1\rangle\langle g_1| = XX^\dagger + YY^\dagger$

with constraint $XY^\dagger = 0$ from strong orthog.

constrained version Weyl's prob, $A = XX^\dagger$, $B = YY^\dagger$, $C = LHS$

General case, constraints more complex to write out

Aside

Klyachko (2005) announced sol'n of pure state N-rep of 1-matrix

Recovers Borland-Dennis conditions for $N = 3, R = 6$

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1 \qquad \lambda_k \text{ dec.}$$

and $\lambda_1 + \lambda_2 \leq \lambda_3 + 1$

Klyachko remarked no progress for over 30 years since.

Ruskai unpublished – use Coleman double induct to prove $= 1$ part

proof of $\lambda_1 + \lambda_2 \leq \lambda_3 + 1$ reduce to Weyl's problem for 2×2

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Aside on SVD and “Schmidt” decomposition

Singular Value Decomposition: Recall $B^*B = \sum_k \mu_k^2 |b_k\rangle\langle b_k| \equiv |B|^2$

Then $B = U|B| = \sum_k \mu_k |a_k\rangle\langle b_k| \qquad |a_k\rangle = U|b_k\rangle$

U partial isometry – restriction to $(\ker B)^\perp$ unique unitary

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Isomorphism $\mathcal{B}(\mathcal{H}) \simeq \mathcal{H} \otimes \mathcal{H} \qquad |v\rangle\langle w| \leftrightarrow |v \otimes w\rangle$

apply SVD + iso to $|\psi\rangle \in \mathcal{H} \otimes \mathcal{H} \qquad |\psi\rangle = \sum_k \mu_k |\alpha_k \otimes \beta_k\rangle$

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pure $\rho_{AB} = |\psi\rangle\langle\psi| \Rightarrow$ reduced density matrices $\rho_A \equiv \mathrm{Tr}_B\, \rho_{AB}$ etc.

$$\rho_A = \sum_k |\mu_k|^2 |\alpha_k\rangle\langle\alpha_k| \quad \rho_B = \sum_k |\mu_k|^2 |\beta_k\rangle\langle\beta_k|$$

Cor: $\rho_{AB} = |\psi\rangle\langle\psi|$ pure $\Rightarrow \rho_A, \rho_B$ have same non-zero e-vals

Can reverse to get "purification" start with $\rho = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$

Define $|\psi\rangle = \sum_k \sqrt{\lambda_k}\, |\phi_k \otimes \phi_k\rangle \in \mathcal{H} \otimes \mathcal{H} \qquad \mathrm{Tr}_B |\psi\rangle\langle\psi| = \rho$

some view: mystical result of Schmidt about tensor products

SVD for matrices back to 1870's (R. Horn & C. Johnson, Chap. 3)

Schmidt(1907) equiv. result interp $K(x, y)$ as kernal of op.

$$g(y) \mapsto f(x) = \int K(x, y) g(y) dy$$

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John Coleman (1963) pointed out due to Schmidt

OK interp $\psi(x,y) = \psi(x_1 \dots x_m, y_1 \dots y_n) \in L_2(\mathbf{R}^{m+n})$ wave func.

can not really expect extension to higher order tensor products

by same iso would also apply to maps $\mathcal{H}^{\otimes m} \mapsto \mathcal{H}^{\otimes n}$

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More info: See Appendix A of King and Ruskai

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Aside on group representation terminology

Connect reps of $SU(n)$ and S_n $\quad \mathbf{C}_d^{\otimes n} = \bigoplus_\lambda U_\lambda \otimes V_\lambda$

For any group $\quad R_\lambda \times R_\mu = \sum_\nu g_{\lambda\mu\nu} R_\nu$

The coefficients $g_{\lambda\mu\nu}$ called

For $SU(n)$ Littlewood-Richardson coefficients (math)

or Clebsch-Gordon coefficients (physics)

Symmetric group S_n Kronecker coefficients

duality leads to sol'n of Weyl's prob in terms of coef. for $SU(n)$

sol'n of quant marg prob in terms of coef. for S_n

discussed in Christandl's talk

Open Problem 1

- N-rep for 1-matrix depends only on eigenvalues
- N-rep for 2-matrix also depends on eigenvectors

In gen, N-rep conds don't depend on choice of 1-particle basis

N-rep conditions for m-matrix can be expressed in terms of

quantities invariant under unitaries of form $U^{\otimes m}$

$U \otimes U \otimes \ldots \otimes U$ called "local unitaries" in quantum info

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Challenge: Find a "full, minimal" set of invariants for 2-matrix?

Open Problem 2

Can Klyachko's results for pure N-rep of one-matrix

possibly combined with Ando-Coleman Theorem

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but actually 4 will suffice

can one reduce number of coeffs in CI in other situations?

Klyachko ineq assume arbitrary coeff, but might give hints

Can reduce effective R, N by assuming some $\lambda_k = 1$?

When is this a good approximation?

Open Problem 3: Conjectured gen of A. Horn's Lemma

Φ is quantum channel or completely pos, trace-pres (CPT) map

Conj 1: Let $\Phi : M_{d_1} \mapsto M_{d_2}$ be a CPT map. Then $\exists$ d_2 CPT maps Φ_m with Choi rank $\leq d_1$ such that $\Phi = \sum_{m=1}^{d_2} \frac{1}{d_2} \Phi_m$.

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Conj 2: Let $\Phi : M_{d_2} \mapsto M_{d_1}$ be a CP map with $\Phi(I_2) = I_1$. Then $\exists$ d_2 unital CP maps Φ_m with Choi rank $\leq d_1$ s.t. $\Phi = \sum_{m=1}^{d_2} \frac{1}{d_2} \Phi_m$

Conjectures of K.M.R. Audenaert and M.B. Ruskai
strongly supported by numerical work of Audenaert

Can prove for $d_1 = 1$ or $d_2 = 2$ using block matix version.

Using only true extreme points need up to $d_1 d_2$ maps

Block Matrix forms of Audenaert-Ruskai conjecture

Conj 3: Let $\mathbf{A}$ be a $d_1 d_2 \times d_1 d_2$ pos semi-def. matrix with $d_2 \times d_2$ blocks A_{jk} each $d_1 \times d_1$, with $\sum_j A_{jj} = M$. $\exists$ d_2 block matrices $\mathbf{B}_m$, each of rank $\leq d_1$, s.t. $\sum_j B_{jj} = M$, and $\mathbf{A} = \sum_{m=1}^{d_2} \frac{1}{d_2} \mathbf{B}_m$.

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Conj 3: Let $\mathbf{A}$ be a $d_1 d_2 \times d_1 d_2$ pos semi-def. matrix with $d_2 \times d_2$ blocks A_{jk} each $d_1 \times d_1$, with $\sum_j A_{jj} = M$. $\exists$ d_2 block matrices $\mathbf{B}_m$, each of rank $\leq d_1$, s.t. $\sum_j B_{jj} = M$, and $\mathbf{A} = \sum_{m=1}^{d_2} \frac{1}{d_2} \mathbf{B}_m$.

Restate using vectors of matrices $\mathbf{X}_m^\dagger = \begin{pmatrix} X_{1m}^\dagger & X_{2m}^\dagger & \ldots & X_{d_2 m}^\dagger \end{pmatrix}$ with each block X_{jm} $d_1 \times d_1$.

Conj 4: Let $\mathbf{A}$ be a $d_1 d_2 \times d_1 d_2$ pos semi-def. matrix with $d_2 \times d_2$ blocks A_{jk} each $d_1 \times d_1$, with $\sum_j A_{jj} = M$. Then $\exists$ d_2 vectors $\mathbf{X}_m$ composed of d_2 blocks X_{jm} of size $d_1 \times d_1$ such that

$$\mathbf{A} = \sum_{m=1}^{d_2} \frac{1}{d_2} \mathbf{X}_m \mathbf{X}_m^\dagger, \qquad \text{and} \qquad \sum_k X_{km} X_{km}^\dagger = M \qquad \forall\ m$$

Horn's Lemma and Corollary

Def: For sequences $\{a_k\}, \{b_k\}$ of length n in non-increasing order, a_k majorizes b_k, written $a_k \succ b_k$ means

$$a_1 \geq b_1 \qquad \sum_{k=1}^{m} a_k \geq \sum_{k=1}^{m} b_k \qquad \sum_{k=1}^{n} a_k = \sum_{k=1}^{n} b_k$$

Horn's Lemma: Given positive sequences $\{\lambda_k\}, \{d_k\}$ of length n, there exists a positive semi-definite $n \times n$ matrix A with e-vals λ_k and diagonal elements d_k if and only if $\lambda_k \succ d_k$.

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Any seq of n els with $\lambda_k \geq 0$ and $\sum_k \lambda_k = 1$ majorizes $d_k = \frac{1}{n}$

Cor: Let A be a $n \times n$ pos semi-def matrix with $\mathrm{Tr}\, A = 1$. Then $\exists$

n normalized (not nec orthog) vectors $\mathbf{x}_m$ s. t. $A = \sum_{m=1}^{n} \frac{1}{n} \mathbf{x}_m \mathbf{x}_m^\dagger$

See Ruskai, arXiv:0708.1902 Some Open Problems in Quant Info.

Open Problem 4:

Most interesting when $v \not\succ w$

Answer #1 there is a z such that $v \otimes z \succ v \otimes w$

Answer #2 there is an n such that $v^{\otimes n} \succ w^{\otimes n}$

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Is there a natural question in Schubert calculus framework?