The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

2044-9

Summer School and Advanced Workshop on Trends and Developments in Linear Algebra

22 June - 10 July, 2009

Matrix analysis quantum theory

Dénes Petz

Hungarian Academy of Sciences
Budapest
Hungary

---

petz@math.bme.hu
http://www.renyi.hu/~petz

Matrix analysis $\bigcap$ quantum theory

Dénes Petz

Alfréd Rényi Institute of Mathematics
Hungarian Academy of Sciences

E-mail: petz@math.bme.hu **Home page:** http://www.renyi.hu/~ petz

Density matrices

In the mathematical formalism of quantum mechanics, instead of n-tuples of numbers one works with $n \times n$ complex matrices.

They form a non-commutative algebra and this allows an algebraic approach.

In this approach, a probability density is replaced by a positive semidefinite matrix of trace 1 which is called **density matrix**.

Statistical operator is an alternative terminology.

The eigenvalues of a density matrix give a probability density.

Entropies

Von Neumann entropy (von Neumann, 1927):

$$S(D) := -\mathrm{T}r D \log D$$

Relative entropy (Umegaki, 1962):

$$S(D_1 \| D_2) := \mathrm{T}r D_1 (\log D_1 - \log D_2)$$

Here the functional calculus is used. If D_1 and D_2 commute, then the relative entropy is the same as in the classical case.

Old results

Theorem (von Neumann, 1932): If $f : \mathbb{R} \hookrightarrow \mathbb{R}$ is concave, then $A \mapsto \mathrm{Tr} f(A)$ is concave.

Corollary: The von Neumann entropy is concave.

Theorem (Klein $\to$ DP): If $f_i, g_i : \mathbb{R} \hookrightarrow \mathbb{R}$ and

$$\sum_i f_i(x) g_i(y) \geq 0, \quad \text{then} \quad \sum_i \mathrm{Tr} f_i(A) g_i(B) \geq 0.$$

Corollary (Streater, 1985):

$$S(D_1 \| D_2) \geq \frac{1}{2} \mathrm{Tr}(D_1 - D_2)^2 + \mathrm{Tr} D_1 - \mathrm{Tr} D_2$$

Development

Theorem (Lieb concavity, 1973): If $0 < t < 1$f, then

$$0 \leq A \mapsto \mathrm{Tr} A^t K A^{1-t} K^*$$

is concave.

Relative modular operator (cca. 1980):

$$\Delta(D_2, D_1)X = D_2 X D_1^{-1}$$

Quasi-entropy (DP, 1986): $f : \mathbb{R}^+ \to \mathbb{R}$

$$S_f^K(D_1, D_2) := \langle K D_1^{1/2}, f(\Delta(D_2, D_1)) K D_1^{1/2} \rangle,$$

where $\langle\ ,\ \rangle$ is the Hilbert-Schmidt inner product.

Quasi-entropy is jointly concave $\to$ Lieb concavity. Relative entropy is quasi-entropy.

Monotonicity of quasi-entropy

Let $\alpha : \mathcal{M}_0 \to \mathcal{M}$ be a mapping between two matrix algebras. The dual $\alpha^* : \mathcal{M} \to \mathcal{M}_0$ with respect to the Hilbert-Schmidt inner product is positive if and only if α is positive.

$\alpha : \mathcal{M}_0 \to \mathcal{M}$ is called a **Schwarz mapping** if

$$\alpha(B^*B) \geq \alpha(B^*)\alpha(B) \qquad (B \in \mathcal{M}_0).$$

Theorem 1 *Assume that $f : \mathbb{R}^+ \to \mathbb{R}$ is an operator monotone function with $f(0) \geq 0$ and $\alpha : \mathcal{M}_0 \to \mathcal{M}$ is a unital Schwarz mapping. Then*

$$S_f^K(\alpha^*(\rho_1), \alpha^*(\rho_2)) \geq S_f^{\alpha(K)}(\rho_1, \rho_2)$$

holds for $K \in \mathcal{M}_0$ and for invertible density matrices ρ_1 and ρ_2 from the matrix algebra $\mathcal{M}$.

Reduced density

D_{12} is a density matrix in $M_n \otimes M_m$. If $A \leftrightarrow A \otimes I_m$, then $M_n \subset M_n \otimes M_m$.

The reduced density D_1 is defined by

$$\mathrm{Tr} D_{12}(A \otimes B) = (\mathrm{Tr} D_1 A) \mathrm{Tr} B \qquad (A \in M_n, B \in M_m)$$

(Physicists notation $D_1 = \mathrm{Tr}_2 D$, partial trace.)

Example: Let

$$D_{12} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \in M_2 \otimes M_n.$$

Then

$$D_1 = \begin{bmatrix} \mathrm{Tr} A_{11} & \mathrm{Tr} A_{12} \\ \mathrm{Tr} A_{21} & \mathrm{Tr} A_{22} \end{bmatrix}, \qquad D_2 = A_{11} + A_{22}.$$

Strong subadditivity of entropy

(Lieb-Ruskai 1973)

$$S(D_{123}) + S(D_2) \leq S(D_{12}) + S(D_{23}),$$

where D_{123} is a density in $M_k \otimes M_m \otimes M_n$ and D_{12}, D_2, D_{23} are reduced densities. Equivalalent form:

$$S(D_{12} \| D \otimes D_2) \leq S(D_{123} \| D \otimes D_{23})$$

This is a particular case of monotonicity,

$$\alpha : M_k \otimes M_m \to M_k \otimes M_m \otimes M_n$$

is the embedding.

What is the necessary and sufficient condition for the equivality?

(This is related to sufficient statistics.)

Equality in monotonicity

If $C_{12}, D_{12} \in M_m \otimes M_n$ and C_1, D_1 are the reduced densities, then

$$S(C_1 \| D_1) \le S(C_{12} \| D_{12})$$

holds. This is a particular case of the monotonicity thm, but enough for the proof of the SSA.
Conditions for equality (DP 1986, also in the setting of von Neumann algebras) are the following:

1. $C_1^{\mathrm{it}} D_1^{-\mathrm{it}} = C_{12}^{\mathrm{it}} D_{12}^{-\mathrm{it}}$ for every real t

2. $C_{12}^{\mathrm{it}} D_{12}^{-\mathrm{it}} \in M_m$ for every real t

3. $\log C_1 - \log D_1 = \log C_{12} - \log D_{12}$,

Markov property

The following conditions are equivalent.

1. $S(D_{123}) - S(D_{23}) = S(D_{12}) - S(D_2)$

2. $D_{123}^{\mathrm{it}} D_{23}^{-\mathrm{it}} = D_{12}^{\mathrm{it}} D_2^{-\mathrm{it}}$ for every real t,

3. $D_{123}^{1/2} D_{23}^{-1/2} = D_{12}^{1/2} D_2^{-1/2}$

4. $\log D_{123} - \log D_{23} = \log D_{12} - \log D_2$

5. $D_{123} = XZ, \quad D_{23} = YZ$, where Z commutes with X and Y, moreover X and Y are in the algebra generated by the operators $D_{123}^{\mathrm{it}} D_{23}^{-\mathrm{it}}$.

Remark: $D_{123} D_{23}^{-1} = D_{12} D_2^{-1}$ is weaker.

Problem: What about $D_{123}^{n} D_{23}^{-n} = D_{12}^{n} D_2^{-n}$ for all $n \in \mathbb{Z}$?

Golden-Thompson inequality

Theorem (Golden, Thompson, 1965) For self-adjoint $A, B \in M_n$

$$\mathrm{Tr} e^{A+B} \le \mathrm{Tr} e^A e^B.$$

(DP, 1994) Equality iff $AB = BA$.

Theorem (Lieb, 1973) For self-adjoint $A, B, C \in M_n$

$$\mathrm{Tr} e^{A+B+C} \le \int_0^\infty \mathrm{Tr} (t + e^{-A})^{-1} e^B (t + e^{-A})^{-1} e^C \, dt.$$

My problem: Give a new proof and find the equality condition.

Application to SSA

The operator

$$\exp(\log D_{12} - \log D_2 + \log D_{23})$$

is positive and can be written as $\lambda\omega$ for a density matrix ω. We have

$$\begin{aligned} S(D_{12}) + S(D_{23}) - S(D_{123}) - S(D_2) \\ &= \mathrm{T}r D_{123} \left(\log D_{123} - (\log D_{12} - \log D_2 + \log D_{23})\right) \\ &= S(D_{123} \| \lambda\omega) = S(D_{123} \| \omega) - \log \lambda \end{aligned}$$

Therefore, $\lambda \leq 1$ implies the positivity of the left-hand-side (and the strong subadditivity).

Application to SSA (2)

Due to the Golden-Thompson-Lieb inequality, we have

$$\mathrm{Tr}\exp(\log D_{12} - \log D_2 + \log D_{23})$$

$$\le \int_0^\infty \mathrm{Tr} D_{12}(tI + D_2)^{-1} D_{23}(tI + D_2)^{-1}\, dt$$

Applying the partial traces we have

$$\mathrm{Tr} D_{12}(tI+D_2)^{-1} D_{23}(tI+D_2)^{-1} = \mathrm{Tr} D_2(tI+D_2)^{-1} D_2(tI+D_2)^{-1}$$

and that can be integrated out. Hence

$$\int_0^\infty \mathrm{Tr} D_{12}(tI + D_2)^{-1} D_{23}(tI + D_2)^{-1}\, dt = \mathrm{Tr} D_2 = 1.$$

and $\lambda \le 1$. This gives the strong subadditivity.

Equality in SSA

If the equality holds in the SSA, then
$\exp(\log D_{12} - \log D_2 + \log D_{23})$ is a density matrix and

$$S(D_{123} \| \exp(\log D_{12} - \log D_2 + \log D_{23})) = 0$$

implies

$$\log D_{123} = \log D_{12} - \log D_2 + \log D_{23}.$$

This is the necessary and sufficient condition for the equality.

Proof is due to József Pitrik, see

- D. Petz, *Quantum Information Theory and Quantum Statistics*, Springer, Berlin, Heidelberg, 2008.

Gaussian random triplet

$\mathbf{X}_1$, $\mathbf{X}_2$ and $\mathbf{X}_3$ are random vectors with Gaussian joint distribution

$$f(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \sqrt{\frac{\mathrm{Det} M}{(2\pi)^n}} \exp\Big(- \tfrac{1}{2} \langle \mathbf{x}, M\mathbf{x} \rangle \Big),$$

where the **quadratic matrix** M is $3n \times 3n$ or a 3×3 block matrix:

$$M = \begin{bmatrix} A_1 & A_2 & B_1 \\ A_2^* & A_3 & B_2 \\ B_1^* & B_2^* & D \end{bmatrix}$$

Let the distribution of the appropriate marginals be $f(\mathbf{x}_1, \mathbf{x}_2)$, $f(\mathbf{x}_2, \mathbf{x}_3)$ and $f(\mathbf{x}_2)$.

Gaussian Markov triplet

(Ando-DP, 2008) Equivalent conditions:

(1) $f(\mathbf{x}_3|\mathbf{x}_1, \mathbf{x}_2) = f(\mathbf{x}_3|\mathbf{x}_2)$

(2) $B_1 = 0.$

(3) The conditional distribution $f(\mathbf{x}_3|\mathbf{x}_1, \mathbf{x}_2)$ does not depend on $\mathbf{x}_1$.

(4) The covariance matrix of $(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)$ is of the form

$$M^{-1} = \begin{bmatrix} S_{11} & S_{12} & S_{12}S_{22}^{-1}S_{23} \\ S_{12}^* & S_{22} & S_{23} \\ S_{23}^*S_{22}^{-1}S_{12}^* & S_{23}^* & S_{33} \end{bmatrix}$$

(5) $h(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) - h(\mathbf{X}_2, \mathbf{X}_3) = h(\mathbf{X}_1, \mathbf{X}_2) - h(\mathbf{X}_2)$, where h denotes the Boltzmann-Gibbs entropy.

CCR-algebra

Let $\mathcal{H}$ be a finite dimensional Hilbert space. Assume that for every $f \in \mathcal{H}$ a unitary operator $W(f)$ is given such that the relations

$$W(f_1)W(f_2) = W(f_1 + f_2)\exp(\mathrm{i}\,\sigma(\mathrm{f}_1, \mathrm{f}_2))$$

and

$$W(-f) = W(f)^*$$

hold for $f_1, f_2, f \in \mathcal{H}$ with $\sigma(f_1, f_2) := \mathrm{Im}\langle f_1, f_2\rangle$.
The C*-algebra generated by these unitaries is unique and denoted by $\mathrm{CCR}(\mathcal{H})$.

$$CCR(\mathcal{H}_1 \oplus \mathcal{H}_2) = CCR(\mathcal{H}_1) \otimes CCR(\mathcal{H}_2)$$

Quasi-free state

For $0 \leq A \in B(\mathcal{H})$ set

$$\omega_A(W(f)) := \exp\big(- \|f\|^2/2 - \langle f, Af \rangle\big).$$

Assume that $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ and write the positive mapping $A \in B(\mathcal{H})$ in the form of block matrix:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}.$$

If $f \in \mathcal{H}_1$, then

$$\omega_A(W(f \oplus 0)) = \exp\big(- \|f\|^2/2 - \langle f, A_{11} f \rangle\big).$$

Therefore the restriction of the quasi-free state ω_A to $\mathrm{CCR}(\mathcal{H}_1)$ is the quasi-free state $\omega_{A_{11}}$.

Quasi-free state (2)

Let the spectral decomposition of $0 \leq A \in B(\mathcal{H})$ be

$$A = \sum_{i=1}^{m} \lambda_i |e_i\rangle\langle e_i|.$$

Then the von Neumann entropy of the quasi-free state ω_A is

$$S(\omega_A) = \mathrm{T}r\eta(A) - \mathrm{T}r\eta(A+I),$$

where $\eta(t) = -t \log t$.

Remark: The function $\kappa(x) := -x \log x + (x+1)\log(x+1)$ is matrix monotone.

Markov triplet

Let $CCR(\mathcal{H}) = CCR(\mathcal{H}_1) \otimes CCR(\mathcal{H}_2) \otimes CCR(\mathcal{H}_3)$, where $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3$ and let ω_{123} be a quasi-free state. Then

$$\omega_{123} \leftrightarrow \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}, \qquad \omega_2 \leftrightarrow [\, A_{22} \,],$$

$$\omega_{12} \leftrightarrow \begin{bmatrix} A_{11} & A_{12} & \\ A_{21} & A_{22} & \end{bmatrix}, \qquad \omega_{23} \leftrightarrow \begin{bmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{bmatrix}$$

Definition:

$$S(\omega_{123}) - S(\omega_{23}) = S(\omega_{12}) - S(\omega_1)$$

Block matrices

Theorem. (Jenčova-DP-Pitrik, 2008) For a quasi-free state ω_A the Markov property is equivalent to the condition

$$A^{\mathrm{it}}(I+A)^{-\mathrm{it}}D^{-\mathrm{it}}(I+D)^{\mathrm{it}} = B^{\mathrm{it}}(I+B)^{-\mathrm{it}}C^{-\mathrm{it}}(I+C)^{\mathrm{it}}$$

for every real t, where

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}, \quad D = \begin{bmatrix} I & 0 & 0 \\ 0 & A_{22} & A_{23} \\ 0 & A_{32} & A_{33} \end{bmatrix}$$

and

$$B = \begin{bmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} & 0 \\ 0 & 0 & I \end{bmatrix}, \quad C = \begin{bmatrix} I & 0 & 0 \\ 0 & A_{22} & 0 \\ 0 & 0 & I \end{bmatrix}.$$

Example and result

Proof idea: Von Neumann entropy formula and second quantization.

Example: The following matrix satisfies the Markov condition.

$$A = \begin{bmatrix} A_{11} & \begin{bmatrix} a & 0 \end{bmatrix} & 0 \\ \begin{bmatrix} a^* \\ 0 \end{bmatrix} & \begin{bmatrix} c & 0 \\ 0 & d \end{bmatrix} & \begin{bmatrix} 0 \\ b \end{bmatrix} \\ 0 & \begin{bmatrix} 0 & b^* \end{bmatrix} & A_{33} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} A_{11} & a \\ a^* & c \end{bmatrix} & 0 \\ 0 & \begin{bmatrix} d & b \\ b^* & A_{33} \end{bmatrix} \end{bmatrix},$$

where the parameters a, b, c, d (and 0) are matrices.

Theorem. (Jenčova-DP-Pitrik, 2008) This is the only possibility.

References

- D. Petz, Quasi-entropies for finite quantum systems, Rep. Math. Phys., **23**(1986), 57-65.
- D. Petz, Sufficient subalgebras and the relative entropy of states of a von Neumann algebra, Commun. Math. Phys. **105**(1986), 123–131.
- M. Ohya and D. Petz, *Quantum Entropy and Its Use*: Springer-Verlag, Heidelberg, 1993. Second edition 2004.
- D. Petz, Monotone metrics on matrix spaces, Linear Algebra Appl. **244**(1996), 81–96.

Recent references

- A. Jenčova and D. Petz, Sufficiency in quantum statistical inference, Commun. Math. Phys. **263**(2006), 259–276.
- D. Petz, *Quantum Information Theory and Quantum Statistics*, Springer, Berlin, Heidelberg, 2008.
- A. Jenčova, D. Petz and J. Pitrik, Markov triplets on CCR-algebras, to be published in Acta Szeged.
- T. Ando and D. Petz, Gaussian Markov triplets approached by block matrices, Acta Sci. (Szeged) **75**(2009), 265–281.