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An alternative approach to Quantum Information Geometry

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Contents

This talk is based on the content of the following papers.

[1] J. Naudts, Quantum Statistical Manifolds, Entropy 20, 472 (2018), correction 20, 796 (2018).

[2] J. Naudts, Log-affine geodesics in the manifold of vector states on a von Neumann algebra, submitted to J. Math. Phys; arXiv:1901.06267v3 (2019).

[3] J. Naudts, Quantum statistical manifolds: The linear growth case, to appear in Rep. Math. Phys.; arXiv:1801.07642v2 (2019).

Part I

The alternative

I.1 von Neumann Algebras

A von Neumann algebra is an algebra of operators on a complex Hilbert space $\mathcal{H}$; This algebra should satisfy some additional requirements

EXAMPLE The algebra of all $n \times n$ matrices

EXAMPLE The algebra of all bounded operators on a complex Hilbert space

EXAMPLE The Banach algebra L^∞ of essentially bounded measureable functions on $\mathbb{R}^n, \mathrm{d}x$

Quantum mechanics

The probability distribution over $\{x_1, x_2, \cdots x_n\}$ can be written as

$$\rho = \begin{pmatrix} p_1 & 0 & \cdots & 0 \\ 0 & p_2 & \cdots & 0 \\ & & \cdots & \\ 0 & 0 & \cdots & p_n \end{pmatrix} \equiv [p_1, p_2, \cdots p_n].$$

A function f over state space is a diagonal matrix $[f_1, f_2, \cdots f_n]$.

Its expectation value equals $\mathbb{E}\, f = \mathrm{Tr}\, \rho f = \sum_j p_j f_j$.

ρ is a *density matrix* in diagonal form.

In quantum mechanics ρ and f may be non-diagonal.

$\mathbb{E}\, f = \mathrm{Tr}\, \rho f$ still gives the expectation of the matrix f.

States

STATISTICS

Our interest is in expectation values
They define a *state* ω of
the von Neumann algebra $\mathcal{A}$

A state is a complex linear function $\omega : \mathcal{A} \mapsto \mathbb{C}$

- $\omega(\mathbb{I}) = 1$;
- $A \geq 0$ implies $\omega(A) \geq 0$;

THEOREM   Any state ω of $\mathcal{A}$ belongs to the dual $\mathcal{A}^*$

EXAMPLE $\omega(A) = (A\Omega, \Omega)$
where Ω is a normalized vector in $\mathcal{H}$
This is called a vector state

EXAMPLE $\omega(A) = \mathrm{Tr}\,\rho A$ where ρ is a density matrix

EXAMPLE $\omega(f) = \int f(x)|\psi(x)|^2\,\mathrm{d}x$
where $\psi(x)$ is square integrable
This is a vector state on L^∞

The GNS representation

GNS THEOREM (Gelfand-Naimark-Segal)
For each state ω on a C^*-algebra there exists a representation as operators on a Hilbert space $\mathcal{H}$ such that $\omega(A) = (A\Omega, \Omega)$ for some Ω in $\mathcal{H}$.

Note: A von Neumann algebra is always a C^*-algebra

Note: A Radon probability measure can be defined as a state on the C^*-algebra of continuous functions with compact support in a locally compact Hausdorff space

Two representations of a matrix A

$n \times n$ matrix represented as $n^2 \times n^2$ matrices in two ways

$$\begin{pmatrix} A & 0 & \cdots & 0 \\ 0 & A & \cdots & 0 \\ & & \cdots & \\ 0 & 0 & \cdots & A \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} a_{1,1}\mathbb{I} & a_{1,2}\mathbb{I} & \cdots & a_{1,n}\mathbb{I} \\ a_{2,1}\mathbb{I} & a_{2,2}\mathbb{I} & \cdots & a_{2,n}\mathbb{I} \\ & & \cdots & \\ a_{n,1}\mathbb{I} & a_{n,2}\mathbb{I} & \cdots & a_{n,n}\mathbb{I} \end{pmatrix}$$

In tensor product notation $A \otimes \mathbb{I}$ and $\mathbb{I} \otimes A$

The two representations commute
$(A \otimes \mathbb{I})\,(\mathbb{I} \otimes B) = (A \otimes B) = (\mathbb{I} \otimes B)\,(A \otimes \mathbb{I})$
They generate the algebra $\mathcal{A}$ and its commutant $\mathcal{A}'$

THEOREM If $\mathcal{A}$ is a von Neumann algebra then $\mathcal{A}'' = \mathcal{A}$

In the commutative case is $\mathcal{A} \subset \mathcal{A}'$

Cyclic and separating vectors

The vector Ω of the GNS theorem is *cyclic*:
$\mathcal{A}\Omega = \{A\Omega : A \in \mathcal{A}\}$ is dense in the Hilbert space $\mathcal{H}$

The state ω is *faithful* if $\omega(A^*A) = 0$ implies $A = 0$

ω faithful implies Ω separating: $A\Omega = 0$ with $A \in \mathcal{A}$ implies $A = 0$

THEOREM Ω cyclic and separating for $\mathcal{A} \Leftrightarrow$ for $\mathcal{A}'$

Cyclic and separating vectors are important in Tomita-Takesaki Theory, which exploits the symmetry between a von Neumann algebra and its commutant

I.2 An alternative approach

Fix a non-degenerate density matrix ρ

$\rho\psi_n = p_n\psi_n$ with $p_n > 0$ and $\sum_n p_n = 1$

Construct the GNS representation with

$$\Omega = \sum_n \sqrt{p_n}\, \psi_n \otimes \psi_n$$

Verification:

$$\begin{aligned}(A \otimes \mathbb{I}\,\Omega, \Omega) &= \sum_{m,n} \sqrt{p_m p_n}(A\psi_m \otimes \psi_m, \psi_n \otimes \psi_n) \\ &= \sum_n p_n(A\psi_n, \psi_n) = \mathrm{Tr}\,\rho A.\end{aligned}$$

THEOREM Let ρ, $\mathcal{H}$, Ω be as before. For any other non-degenerate density matrix σ there exists a unique strictly positive operator X in the commutant of $\mathcal{A}$ such that

$$\mathrm{Tr}\,\sigma A = (AX^{1/2}\Omega, X^{1/2}\Omega), \qquad A \in \mathcal{A}$$

This is known since long.

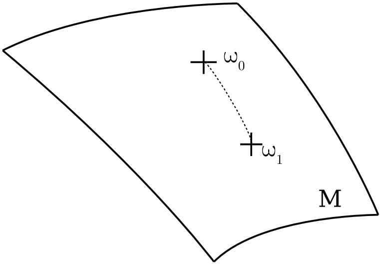
Proof: Define X by $X\,A\Omega = A\sigma\rho^{-1}\Omega$
and verify that X is strictly positive and that

$$(AX^{1/2}\Omega, X^{1/2}\Omega) = (A\sigma\rho^{-1}\Omega, \Omega) = \mathrm{Tr}\,\rho A\sigma\rho^{-1} = \mathrm{Tr}\,\sigma A$$

The Manifold

A manifold of vector states instead of a manifold of density matrices ...

Since states belong to the dual Banach space $\mathcal{A}^*$ also tangent vectors belong to it.



$\mathbb{M}$ denotes a manifold of vector states on $\mathcal{A}$ and select a state ω_0 in $\mathbb{M}$ with corresponding vector Ω_0.

Assume that Ω_0 is cyclic and separating for $\mathcal{A}$.

A geodesic connecting a state ω_1 in $\mathbb{M}$ to the state ω_0 is a map $s \in [0, 1] \mapsto \omega_s \in \mathbb{M}$ satisfying some properties.

The tangent vector f_s at the point ω_s is given by $f_s = \dfrac{\mathrm{d}\omega_s}{\mathrm{d}s}$. assuming that the derivative exists as an element of $\mathcal{A}^*$.

Logarithmic derivatives

Needed is $f_s(A) = \frac{\mathrm{d}}{\mathrm{d}s}(AX_s^{1/2}\Omega_0, X_s^{1/2}\Omega_0)$
with $\Omega_s = X_s^{1/2}\Omega_0$.

Assume $X_s = \exp(\log X_0 + sH)$.

Then classically

$$\frac{\mathrm{d}}{\mathrm{d}s}\exp\left(\frac{1}{2}\log X_0 + \frac{s}{2}H\right) = \frac{1}{2}H\exp\left(\frac{1}{2}\log X_0 + \frac{s}{2}H\right) \quad (*).$$

Quantum problem: H does not commute with X_0.
Hence, (*) is NOT valid.

DEFINITION The *left logarithmic derivative* of $s \mapsto Q_s$ is any solution of

$$\frac{\mathrm{d}}{\mathrm{d}s} Q_s = L_s Q_s$$

- See D. Petz, G. Toth, The Bogoliubov inner product in quantum statistics, Lett. Math. Phys. 27, 205–216 (1993).

- The Physics Literature uses a symmetric logarithmic derivative.

Let $Q_s = X_s^{1/2}$ with $X_s = \exp(\log X_0 + sH)$

Abelian case: $L_s = \frac{1}{2} H$

Matrix algebra: $L_s = \frac{1}{2} \int_0^1 \mathrm{d}u \, X_s^{u/2} H X_s^{(1-u)/2}$

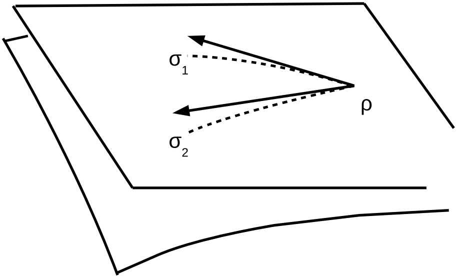
... also valid in the abelian case

The tangent vector f_s satisfies

$$f_s(A) = 2\,(A\Omega_s, L_s\Omega_s)\,, \qquad A \in \mathcal{A}$$

Bogoliubov's inner product

Consider now two density matrices σ_1 and σ_2, besides ρ.



The original version of Bogoliubov's inner product reads

$$g_{1,2} = \int_0^1 \mathrm{d}u \, \mathrm{Tr} \, \rho^u \left[\log \sigma_1 - \log \rho\right] \rho^{1-u} \left[\log \sigma_2 - \log \rho\right]$$

It defines a metric on the tangent plane $T_\rho \mathbb{M}$.

Let $L_0^{(1)}, L_0^{(2)}$ denote the left logarithmic derivatives of

$$X_s^{(1)} = \exp(\log X_0 + sH_1) \text{ and } X_s^{(2)} = \exp(\log X_0 + sH_2).$$

THEOREM (Theorem 6 of my Entropy paper)
There exists an operator $G > 0$ such that

$$g_{1,2} = (G\, L_0^{(1)}\Omega_0, L_0^{(2)}\Omega_0)$$

Other metrics: Wasserstein / Fubini ???

Part II

Symmetries

II.1 Tomita-Takesaki Theory

This theory exploits the symmetry between
a von Neumann algebra $\mathcal{A}$ and its commutant $\mathcal{A}'$
given a cyclic and separating vector Ω_0 in $\mathcal{H}$.

The map $A \otimes \mathbb{I} \mapsto \mathbb{I} \otimes A$ is not so interesting because
the choice of two commuting representations is arbitrary
and the structure of a tensor product
is missing in the general case.

There exists a more intrinsic operator J
satisfying $J = J^*$ and $J^2 = \mathbb{I}$
which maps elements of $\mathcal{A}\Omega_0$ onto elements of $\mathcal{A}'\Omega_0$.

It all started with Tomita's discovery in 1967 that the map

$$A\Omega_0 \mapsto A^*\Omega_0, \qquad A \in \mathcal{A}$$

is closable.

The closure is denoted S; it is an anti-linear operator.
It is called the *modular conjugation operator*.

Any closed linear operator has a polar decomposition.

In this case: $S = J\Delta^{1/2}$ with $\Delta = S^*S$

By von Neumann's theorem the operator Δ is positive
... and hence self-adjoint. It is the *modular operator*.

The operator J is an anti-linear isometry
satisfying $J = J^*$ and $J^2 = \mathbb{I}$.
One has $\Delta\Omega_0 = \Omega_0$ and $J\Omega_0 = \Omega_0$.

THEOREM (Tomita-Takesaki)

— If $A \in \mathcal{A}$ then $\tau_t(A) = \Delta^{-it} A \Delta^{it}$ is in $\mathcal{A}$;

— $A \in \mathcal{A}$ if and only if $JAJ \in \mathcal{A}'$.

$(\tau_t)_t$ is the modular automorphism group

It is the time evolution of Quantum Statistical Physics,
ω_0 is the Gibbs state.

II.2 Labeling States

Plan Use positive operator X affiliated with $\mathcal{A}'$ to label a state ω_X relative to the given state ω_0.

Problem Non-uniqueness: a densily-defined closed operator may have many self-adjoint extensions

Alternative Use a cocycle of the modular automorphism group of ω_0

…explanation follows.

Solutions

— Physicists require that the vectors in the domain of a Hamiltonian satisfy 'boundary conditions';

— von Neumann' s theorem proves that, given a closed operator Y, the operator Y^*Y is self-adjoint on its natural domain of definition;

— Stone's theorem proves that the generator of a strongly-continuous one parameter group $(U_t)_t$ of unitaries has a self-adjoint generator H with domain

$$\left\{ \psi : \left. \frac{\mathrm{d}}{\mathrm{d}t} \right|_{t=0} U_t \psi \text{ converges } \right\};$$

Cocycles

The one parameter group $(U_t)_t$ of unitaries is too restrictive to describe relative motion.
More general is a *cocycle*:

$$U_{s+t} = U_s \tau_s(U_t)$$

Here $(\tau_t)_t$ is the modular automorphism group.

In the abelian case is $\tau_s(U_t) = U_t$ and $(U_t)_t$ is a group.

The cocycle idea is known in Quantum Field Theory as the time evolution of the interaction picture.

A. Connes used the notion of a cocycle to relate the modular automorphism groups of two distinct states.

$t \mapsto U_t \Delta^{-it}$ is a group; By Stone's theorem there exists a positive operator T such that $U_t \Delta^{-it} = T^{it}$.

THEOREM
Assume that Ω_0 is in the domain of $T^{1/2}$.
Then a vector state ω_U is defined by

$$\omega_U(A) = (A\Omega_U, \Omega_U)\,, \quad \text{with} \quad \Omega_U = e^{-\frac{1}{2}\zeta(U)} T^{1/2}\Omega_0.$$

The state ω_U is uniquely determined by the cocycle U.
(Connes, 1973), (Masuda, 1984)

...This is not yet the operator X.

Let Y denote the closure of the map (if closable)

$$A\Omega_0 \mapsto AT^{1/2}\Omega_0, \qquad A \in \mathcal{A}.$$

Let $X = Y^* Y$.
If Y exists then X is positive affilated with $\mathcal{A}'$.

THEOREM
Assume that Ω_0 is in the domain of $ST^{1/2}$.
Then

- $JT^{1/2}\Omega_0 = T^{1/2}\Omega_0$; $(\mathcal{A} \leftrightarrow \mathcal{A}'$ -symmetry)
- Y exists and $Y \subset JT^{1/2}S$;
- $\omega_U(A) = e^{-\zeta(U)}(AX^{1/2}\Omega_0, X^{1/2}\Omega_0)$.

X is uniquely determined by ω_U because

- it is affiliated with the commutant $\mathcal{A}'$;
- $\mathcal{A}\Omega_0$ is a core of Y.

Proof

Assume $\omega(A) = (AY_1\Omega_0, Y_1\Omega_0) = (AY_2\Omega_0, Y_2\Omega_0)$.
Then $AY_1\Omega_0 \mapsto AY_2\Omega_0$ defines an isometry V.
Because $\mathcal{A}\Omega_0$ is a core of Y_1 and of Y_2
this implies that $VY_1 = Y_2$ so that
$X_2 = Y_2^* Y_2 = Y_1^* V^* V Y_1 = Y_1^* Y_1 = X_1$.

II.3 Log-affine geodesics

Consider a one-parameter family of cocycles $s \mapsto (U_t^{(s)})_t$, and corresponding states $\omega_s \equiv \omega_{U^{(s)}}$, operators $T_s, \cdots$.

The geodesic $s \mapsto \omega_s$ is given by

$$\omega_s(A) = e^{-\zeta(s)}(AT_s^{1/2}\Omega_0, T_s^{1/2}\Omega_0) = e^{-\zeta(s)}(AX_s^{1/2}\Omega_0, X_s^{1/2}\Omega_0).$$

PROPOSAL

The map $s \mapsto \omega_s \in \mathbb{M}$ is a *log-affine geodesic* if there exist a self-adjoint operator H and a function $\Phi(s)$ such that

$$[\log T_s + \Phi(s)] - [\log T_r + \Phi(r)] = (s - r)H \quad \text{for all } s, r.$$

Abelian case

In the abelian case is $\Phi(s)$ constant and
$U_t^{(s)} = \exp(istH)$ and $T_s = \exp(sH)$.

DEFINITION

A measurable function $k(x)$ belongs to the *exponential tangent space* at ω_ψ for some $\psi \in L^2(\mathbb{R}^n, \mathbb{C})$ if

$$\int \left[e^{|tk(x)|} - 1\right] \, |\psi(x)|^2 \, \mathrm{d}x < +\infty \quad \text{for some } t \neq 0.$$

Definition 2.14 of (Ay, Jost, Vân Lê, Schwachhöfer, 2017).

THEOREM

Let $h(x) = tk(x)$ where $k(x)$ belongs to the exponential tangent space at ω_ψ.
Assume $h(x)$ is locally square-integrable.
Define a self-adjoint operator H by $(H\phi)(x) = h(x)\phi(x)$.
Let ω_s be the vector state on $\mathcal{A}$ defined by
$\Omega_s = \left[e^{sH-\zeta(s)}\right]^{1/2}\psi$.

Then $s \mapsto \omega_s$ is a log-affine geodesic.

Matrix case

The density matrix of a Quantum Gibbs State is given by (math notation)

$$\rho_\theta = \exp\left(\sum_k \theta^k H_k - \zeta(\theta)\right)$$

with $\zeta(\theta) = \log \mathrm{Tr} \exp(\sum_k \theta^k H_k)$.

Select θ, η and let

$$\rho_s = \exp(\log \rho_\theta + sH - \Phi(s)) \quad \text{with} \quad H = \sum_k (\theta^k - \eta^k) H_k$$

Then $\rho_0 = \rho_\theta$ and $\rho_1 = \rho_\eta$.

THEOREM

$s \mapsto \omega_s$ is a log-affine geodesic which connects ω_η to ω_θ.

Proof

The cocycles are given by $U_t^{(s)} = \rho_s^{-it} \rho_0^{it}$.
The operator T_s is given by $T_s = \Delta \rho_0^{-1} \rho_s$.

Note that $\Delta \rho_0^{-1}$ commutes with ρ_s.
Hence,
$\log T_s = \log \rho_s + \log \Delta \rho_0^{-1} = sH - \Phi(s) + \log \rho_\theta + \log \Delta \rho_0^{-1}$.

$$\log T_s - \log T_r = (s - r)H - \Phi(s) + \Phi(r).$$

This proves the theorem.

$$X_s = S^* \rho_s \otimes \rho_0^{-1} S = J \left[\rho_0^{-1/2} \rho_s \rho_0^{-1/2} \otimes \mathbb{I} \right] J$$

$$\log X_s = J \left[\log \left(\rho_0^{-1/2} \rho_s \rho_0^{-1/2} \right) \otimes \mathbb{I} \right] J = ???$$

CONCLUSION

The assumption that

$$\log X_s = sH - \Phi(s) + \text{ constant operator}$$

is not compatible with the standard notion of
a quantum exponential family.

On the other hand, $\omega_s \mapsto X_s$ is well-defined.

Part III

Deformed logarithms

III.1 The Linear Growth Case

The regularization of exponential growth,
as introduced by (Newton, 2012),
can be described in terms of a deformed logarithm

$$\log_\phi(v) = \int_1^v \frac{1}{\phi(u)}\,\mathrm{d}u \quad \text{with} \quad \phi(u) = \frac{u}{1+u}.$$

One finds

$$\log_\phi(v) = v - 1 + \log v, \qquad v > 0.$$

See (Montrucchio, Pistone, 2017).

The inverse function $\exp_\phi(u)$ grows linearly as $u \uparrow \infty$.

Normalization

$\cdots$ is not trivial in deformed exponential families.

THEOREM (Montrucchio, Pistone, 2017)

Fix a probability measure μ and a pdf p.

- For each μ-integrable function $f(x)$ there exists a unique constant α such that

$$\exp_\phi[f(x) + \log_\phi(p(x)) - \alpha] \cdot \mu(\mathrm{d}x)$$

is again a probability measure.

- The map $f \mapsto \alpha(f)$ is convex.

Non-commutative version

THEOREM

Let Ω be a normalized element of the Hilbert space $\mathcal{H}$.
Let H be a self-adjoint operator on $\mathcal{H}$ such that
Ω is in the domain of $|H|^{1/2}$.

Then there exists a unique $\alpha > 0$ such that
$|| \, [\exp_\phi(H - \alpha)]^{1/2}\Omega|| = 1$.

Convexity of $\alpha(H)$ is missing.

Operator monotonicity

DEFINITION
A real function $f(u)$ is *operator monotone* if

$$A > B \quad \text{implies} \quad f(A) \geq f(B) \qquad \text{for all } A, B \text{ s.a.}$$

The function $f(u) = u - \exp_\phi(u)$ is monotone but not operator-monotone.

Monotonicity can be used to prove convexity of $\alpha(H)$ in the abelian case. It is not sufficient for a general proof.

III.2 Deformed log-affine geodesics

The normalization theorem can be applied to operators T_s as well as X_s!

Operators T_s have symmetry $JT_s^{1/2}\Omega_0 = T_s^{1/2}\Omega_0$.

Operators X_s are affiliated with the commutant $\mathcal{A}'$.

My proposal is to require that $\log_\phi T_s = sH - \alpha(s)$

or more generally $\log_\phi T_s = sH - \alpha(s) + R$?
with R some fixed operator.

Tangent vectors

$\log_\phi X_s = sH - \alpha(s)$ where H is affilated with $\mathcal{A}'$ is assumed in my ROMP paper.

THEOREM

Assume that Ω_0 is in the domain of $|H|^{1/2}$ and that the ω_0-expectation of H vanishes.

— The derivative $\alpha'(s)$ exists;

— $\frac{\mathrm{d}}{\mathrm{d}s} X_s = [H - \alpha'(s)]\, \phi(X_s)$;

— The tangent vectors $f_s = \frac{\mathrm{d}}{\mathrm{d}s} \omega_s$ exist.

Conclusions

- Use T_s instead of X_s — TO BE DONE
- In the abelian case they coincide;
  what is the relation with the works
  of Nigel Newton, of Montrucchio, Pistone?