Attila Andai:

On the curvature of the space of density matrices

Budapest University
of Technology and Economics

Department of Mathematical Analysis

andaia@math.bme.hu

Classical discrete distributions

Base set: $X_n = \{0, \ldots, n\}$ $(n \in \mathbb{N})$.
Distributions on the set X_n can be characterized by n independent parameters

$$p(x, \vartheta_0, \ldots, \vartheta_n) = \vartheta_i, \text{ if } x = i, \quad 0 \le i \le n,$$

where $\vartheta_0 + \cdots + \vartheta_n = 1$.

The 'open' set of distributions on X_n is

$$\mathcal{P}_n = \left\{ (\vartheta_0, \vartheta_1, \ldots, \vartheta_n) \,\middle|\, 0 < \vartheta_i < 1, \sum_{i=0}^{n} \vartheta_i = 1 \right\}.$$

Riemannian metric on $\mathcal{P}_n$

a. Entropy:

The entropy of the distribution $p(x, \vartheta_0, \ldots, \vartheta_n)$ is

$$S(p) = -\sum_{i=0}^{n} p(i) \log p(i) = -\sum_{i=0}^{n} \vartheta_i \log \vartheta_i \ .$$

This function is concave $\rightarrow$ (-1) times its second derivative is a Riemannian metric.

b. Pull back metric from a sphere:

$$\alpha : \mathcal{P}_n \rightarrow \mathbb{S}^n \qquad (\vartheta_0, \ldots, \vartheta_n) \mapsto (\sqrt{\vartheta_0}, \ldots, \sqrt{\vartheta_n}).$$

This map generates a metric on $\mathcal{P}_n$.

c. Fisher information: [Rao, 1945]

$p \in \mathcal{P}_n$, $(1 \leq i, j \leq n)$:

$$g(p)_{ij} := \sum_{k=0}^{n} \frac{1}{p(k,\underline{\vartheta})} \frac{\partial p(k,\underline{\vartheta})}{\partial \vartheta_i} \frac{\partial p(k,\underline{\vartheta})}{\partial \vartheta_j}$$

d. Cencov theorem:

Let us consider the family $(\mathcal{P}_n, g_n)_{n\in\mathbb{N}}$.

If for every Markovian map $\kappa : X_n \times X_m \to \mathbb{R}$

$$g_{\tilde{\kappa}(p)}(\kappa^*(X), \kappa^*(X)) \leq g_p(X, X)$$

$(\forall p \in \mathcal{P}_n, \forall X \in T_p\mathcal{P}_n)$, then the family $(g_n)_{n\in\mathbb{N}}$ is unique.

The geometry of the space $(\mathcal{P}_n, g)$:

Theorem: The metrics a., b., c. and d. are the same.

Corollary: The geometry of the space $(\mathcal{P}_n, g)$ is well-known (curvatures, geodesics, distance, volume).

Noncommutative case

$$\mathcal{P}_n \ni p(x, \vartheta_0, \ldots, \vartheta_n) \;\Leftrightarrow\; \begin{pmatrix} \vartheta_0 & 0 & \ldots & 0 \\ 0 & \vartheta_1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \vartheta_n \end{pmatrix}$$

$$\bigcap$$

$$\mathcal{M}_n^+ \ni D \qquad\qquad \Leftrightarrow\; \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{pmatrix}$$

$\mathcal{M}_n^+$: $n \times n$ self adjoint, positive definite, trace one, complex matrices.

von Neumann entropy:

$$S(p) = -\sum_{k=0}^{n} \vartheta_k \log \vartheta_k \longrightarrow S(D) = -\operatorname{Tr} D \log D \,.$$

Riemannian metrics on the space $\mathcal{M}_n^+$ [$\sim$ 1990]

a. Entropy:
The entropy functional

$$S : \mathcal{M}_n^+ \to \mathbb{R} \quad D \mapsto S(D)$$

is concave $\to$ (-1) times its second derivative is Riemannian metric.

b. Pull back metric from a sphere:

$$\alpha : \mathcal{M}_n^+ \to \mathbb{S}^k \qquad D \mapsto \sqrt{D}$$

This map generates a metric on $\mathcal{M}_n^+$.

c. Fisher-information: ???

d. Cencov theorem $\rightarrow$ Petz theorem [1996]
Let us consider the family $(\mathcal{M}_n^+, K_n)_{n\in\mathbb{N}}$.

Markovian map $\rightarrow$ stochastic map (linear, trace preserving, completely positive).

If for every stochastic map $T : M_n \rightarrow M_m$ the following holds

$$K_{T(D)}(T(X), T(X)) \leq K_D(X, X)$$

$(\forall D \in \mathcal{M}_n^+, \forall X \in T_D\mathcal{M}_n^+)$, then there exists an operator monotone function $f : \mathbb{R}^+ \rightarrow \mathbb{R}$ with the property $f(x) = xf(x^{-1})$, such that

$$K_D(X, Y) = \mathsf{Tr}\left(X \left(R_{n,D}^{\frac{1}{2}} f(L_{n,D} R_{n,D}^{-1}) R_{n,D}^{\frac{1}{2}} \right)^{-1} (Y) \right),$$

where $L_{n,D}$ and $R_{n,D}$ are defined as $L_{n,D}(X) = DX$ and $R_{n,D}(X) = XD$.

These metrics are the noncommutative generalizations of the Fisher-information. (*Monotone metrics*).

a. Entropy:
Monotone metric: $f(x) = \frac{x-1}{\log x}$,
Kubo–Mori metric:

$$K_{\mathrm{KM},D}(X,Y) = \mathrm{Tr} \int_0^\infty (D+t)^{-1} X (D+t)^{-1} Y \; \mathrm{d}\, t \, .$$

b. Pull back metric:
Monotone metric: $f(x) = \frac{(1+\sqrt{x})^2}{4}$,
Wigner–Yanase-metric.

Note: On the set of diagonal matrices these metrics coincide. (Classical case.)

Examples for monotone metrics:
$f_{\mathrm{SM}}(x) = \frac{1+x}{2}$, $f_{\mathrm{LA}}(x) = \frac{2x}{1+x}$, $f_{\mathrm{P1}}(x) = \frac{2x^{p+1/2}}{1+x^{2p}}$ $(0 \leq p \leq 1/2)$, ... (smallest, largest, parametric)

Series expansion of the volume:

Let (M, g) be an n-dimensional Riemannian geometry.

The geodesic ball with center point $p \in M$ with radius R is the following:

$$B_R(p) := \{x \in M \ : \ \text{dist}(p, x) < R\}.$$

For a fixed p point let $V(R)$ denote the volume of $B_R(D)$.

Series expansion of the volume:

Theorem: (*Gray and Vanhecke, 1979; Andai, 2003*) For an n-dimensional Riemannian geometry (M, g), $p \in M$, the series expansion of the volume $V_n(R)$ is

$$V_n(R) = \frac{R^n \pi^{n/2}}{\Gamma\left(\frac{n}{2}+1\right)} \left[1 - \frac{\mathrm{Scal}}{6(n+2)} R^2 + \right.$$

$$+ \frac{-3\|R\|^2 + 8\|\,\mathrm{Ric}\,\|^2 - 5\,\mathrm{Scal}^2 - 18(\Delta\,\mathrm{Scal})}{360(n+2)(n+4)} R^4 +$$

$$\left. + \frac{\text{higher order curvature invariants}}{720(n+2)(n+4)(n+6)} R^6 + O(R^8)\right].$$

Remark: A higher order curvature invariant

$$\sum_{i,j,k,l,m,o,p,q,r,s=1}^{n} (\nabla R)_{ijklm} (\nabla R)_{opqrs} g^{io} g^{jp} g^{kq} g^{lr} g^{ms}.$$

Theorem *(Classical case)* For the Riemannian geometry $(\mathcal{P}_n, g)$ the series expansion of the volume of the geodesic ball is

$$V_n(R) = \frac{r^n \pi^{n/2}}{\Gamma\left(\frac{n}{2}+1\right)} \left[1 - \frac{n(n-1)}{24(n+2)} R^2 + \right.$$

$$+ \frac{n(n-1)(5n-7)}{5760(n+4)} R^4 -$$

$$\left. - \frac{n(n-1)(35n^2-112n+93)}{2903040(n+6)} R^6 + O(R^8)\right].$$

Remark: The elements in the series expansion are independent from the fixed point $p \in M$.

The volume of the geodesic ball around the point p can be written in the form

$$V_n(R) = C_n(R)(1 + \alpha_1 R^2 + \alpha_2 R^4 + \alpha_3 R^6 + O(R^8)),$$

where only the functions α_i depend on the point p.

Note: It is widely believed that the quantity $V(D)$ has *statistical interpretation*. (For example the scalar curvature measures *average statistical uncertainty*.) It is reasonable to expect that more mixed states are less distinguishable than less mixed states. It means mathematically that in this case the scalar curvature of a Riemann structure should have the following monotonicity property: if D_1 is more mixed than D_2 then Scal(D_2) should be smaller then Scal(D_1).

(This is known as Petz conjecture, if the state space is endowed with the Kubo–Mori metric.)

Let us combine this conjecture with the series expansion.

Generalized Petz conjecture: If the state space is endowed with the Kubo–Mori metric and if D_1 is more mixed than D_2 then

$$\alpha_i(D_1) \leq \alpha_i(D_2) \qquad \forall i \in \mathbb{N} .$$

Qubit case

In the simplest quantum case, dealing with 2×2 matrices we can use the Stokes parametrization, that is every state D can be uniquely written in the form

$$D = \frac{1}{2}\Big(I + x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3\Big)\ ,$$

where $(\sigma_i)_{i=1,2,3}$ are the Pauli matrices and $(x_1, x_2, x_3) \in \mathbb{R}^3$ with $x_1^2 + x_2^2 + x_3^2 \le 1$. The interior of the set of states can be identified with the open unit ball in $\mathbb{R}^3$ by this parametrization. For a fixed state $D \in \mathcal{M}_2^+$ (qubit) from the unit ball denote by r the distance from the origin of the state.

Remark: $r = |\lambda_1 - \lambda_2|$; $r = 0$ is the most mixed state, $r = 1$ is a pure state.

Series expansion of the volume:

Smallest metric: $\left(f(x) = \frac{1+x}{2}\right)$
The volume expansion for a fixed $D \in \mathcal{M}_2^+$ qubit is

$$V(R) = \frac{4\pi R^3}{3}\left(1 - \frac{1}{5}R^2 + \frac{2}{105}R^4 - \frac{1}{945}R^6 + O(R^8)\right) .$$

Largest metric: $\left(f(x) = \frac{2x}{1+x}\right)$

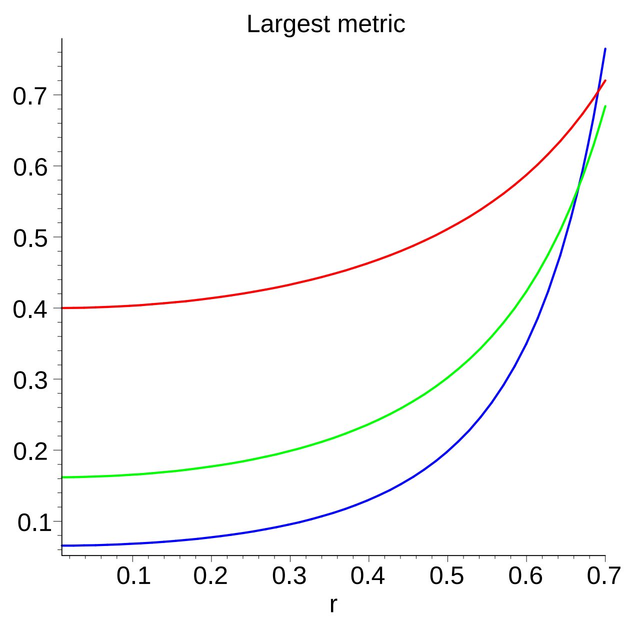
The volume expansion for a fixed $D \in \mathcal{M}_2^+$ qubit is

$$V(R) = \frac{4\pi R^3}{3}\Big(1 - \frac{1}{15}\,\frac{6-r^2}{1-r^2}R^2 +$$

$$+\frac{1}{1575}\,\frac{3r^4+50r^2+225}{(1-r^2)^2}R^4 +$$

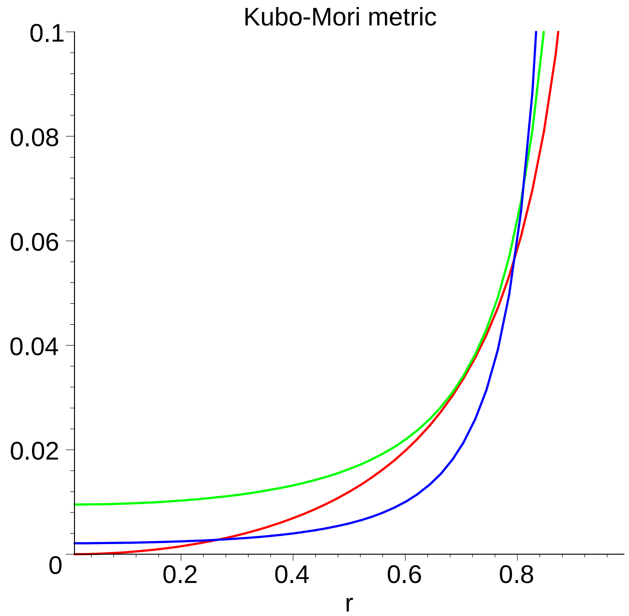
$$+\frac{1}{33075}\frac{r^6-84r^4-2380r^2-2170}{(1-r^2)^3}R^6 + O(R^8)\Big).$$

Let denote the functions α_1, α_2 and α_3 by red, green and blue:



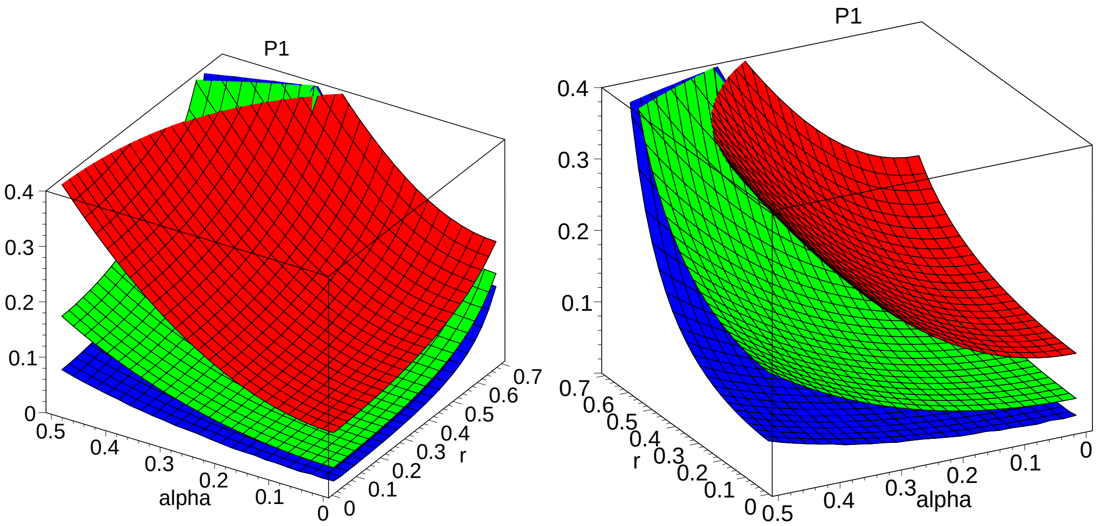
Kubo–Mori-metric: $\left(f(x) = \frac{x-1}{\log x}\right)$

The volume expansion for a fixed $D \in \mathcal{M}_2^+$ qubit can be computed, but the result is a rather complicated formula.



P1 parametric metric: $f(x) = \frac{2x^{p+1/2}}{1+x^{2p}} \left(p \in \left[0, \frac{1}{2}\right]\right)$

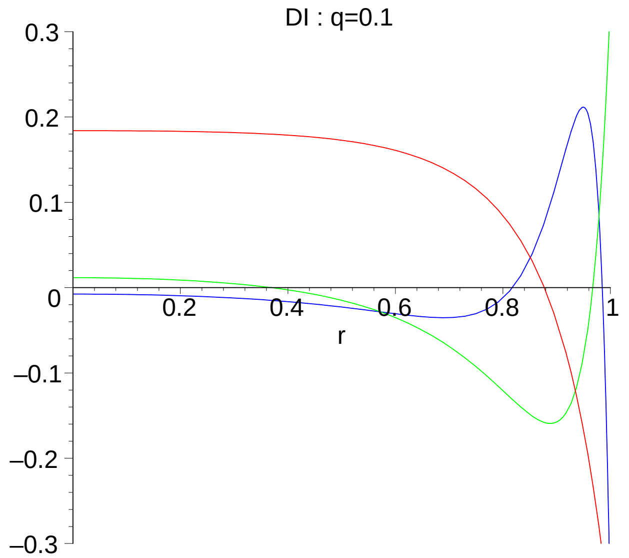
Remark: $\alpha_3(r)$ is the sum of about 500 elements!



If the operator monoton function is

$$f(x) = \frac{9x^2 + 82x + 9}{5(x+1)} \ ,$$

then



Remark: For $n \times n$ density matrices the computing time of the quantities α_i is about n^{20}.

Remark: From the above mentioned cases it seems reasonable that the quantities α_i somehow measures statistical uncertainty. (It was known for α_1.)

Question: What is the behavior of the α_i curvature invariants for higher level quantum systems?