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Summary of the

Information geometry in quantum mechanics

PhD thesis

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1 Introduction

Information geometry began as the geometric study of statistical estimation. This involves viewing the set of probability distributions of a statistical model as a manifold, and analyzing the relationship between the geometric structure of this manifold and statistical estimation. From a mathematical point of view, the non-commutative probability theory, which is appropriate to quantum mechanics, may be constructed as an extension of probability theory, and it is possible to generalize many concepts in probability theory to the non-commutative setting.

The generalization of information geometry to the non-commutative case started in the 90-ies. This area of mathematics applies statistics, differential geometry and functional analysis in order to develop and understand the physical meaning of the non-commutative information geometry. The statistical basis of this area is an information matrix which was introduced by Fisher. Rao suggested to consider this matrix as a Riemannian metric on statistical manifolds in 1945 [16]. In this manner some differential geometrical properties of a statistical manifold has statistical meaning [4]. There are several applications of this method in physics, see for example [10]. This combination of the statistics and differential geometry is called information geometry. The quantum mechanics brought forth the non-commutative probability theory, which is more general then the classical one [12]. In this non-commutative setting, the statistical modell can be considered as a differential manifold, and this manifold can be endowed by Fisher-type Riemannian metrics [13]. This mathematical structure is called as non-commutative information geometry, and there are several application of this structure in quantum physics, see for example [5].

2 Results

The following references concern to the thesis.

1/a. Efron studied first the curvature of the statistical manifolds in 1975 [9]. He found, that the curvature has statistical interpretation. The most well-known statistical model is the family of discrete distributions. For arbitrary $n \in \mathbb{N}$ let $X_n = \{0, \dots, n\}$, the density function $p(x)$ on the set X_n can be represented by n independent variables

$$p(x) = \begin{cases} \vartheta_i & \text{if } x = 1, \dots, n \\ 1 - \sum_{i=1}^n \vartheta_i & \text{if } x = 0. \end{cases} \quad (1)$$

The set of density functions on X_n , which depends on n variables is the following

$$\mathcal{P}_n = \left\{ (\vartheta_1, \dots, \vartheta_n) \mid \forall i \in \{1, \dots, n\} : 0 < \vartheta_i < 1, \sum_{i=1}^n \vartheta_i < 1 \right\}. \quad (2)$$

The set \mathcal{P}_n is a differentiable manifold and the Fisher information matrix defines a Riemannian metric on it. The elements of the metric tensor $g_{ij}^{(F)}$ are the following

$$g_{ij}^{(F)}(\underline{\vartheta}) = \sum_{x=0}^n \frac{1}{p(x, \underline{\vartheta})} \frac{\partial p(x, \underline{\vartheta})}{\partial \vartheta_i} \frac{\partial p(x, \underline{\vartheta})}{\partial \vartheta_j} = \delta_{ij} \frac{1}{\vartheta_i} + \frac{1}{1 - \sum_{k=1}^n \vartheta_k}, \quad (3)$$

where $\underline{\vartheta} = (\vartheta_1, \dots, \vartheta_n) \in \mathcal{P}_n$. So the pair $(\mathcal{P}_n, g^{(F)})$ is a Riemannian geometry, the metric $g^{(F)}$ is called Fisher-metric. For every parameter $\alpha \in [-1, 1]$ there exists an α -connection $\nabla^{(\alpha)}$ on the manifold \mathcal{P}_n . The α -connections were introduced by Cencov in 1982 [6]. (The parameter $\alpha = 0$ corresponds to the Levi-Civita connection.)

The Ricci tensor (Theorem 2.7.) and the scalar curvature (Theorem 2.8.) of the manifold $(\mathcal{P}_n, g^{(F)}, \nabla^{(\alpha)})$ is computed. It is shown that the scalar curvature of the manifold $(\mathcal{P}_n, g^{(F)}, \nabla^{(\alpha)})$ is constant if and only if $\alpha = 0$.

1/b. Gray and Vanhecke computed the Taylor expansion of the volume of a sphere in an arbitrary Riemannian manifold (M, g) in 1979 [11]. Their result is wrong.

I follow they rather long and complicated computation and I give the corrected Taylor expansion of the volume of a sphere (Theorem 2.14.). I give this Taylor expansion in explicit form on the space $(\mathcal{P}_n, g^{(\mathbf{F})})$ (Theorem 2.15.).

2/a. The Fisher information matrix defines a Riemannian metric on the statistical model of the n dimensional normal distributions. For every natural number n let us introduce the following notation

$$M_n^+ = \{D \in M_n(\mathbb{R}) \mid D = D^*, D > 0\} . \quad (4)$$

Every matrix $D \in M_n^+$ determines a normal distribution by the density function

$$f : M_n^+ \times \mathbb{R}^n \rightarrow \mathbb{R} \quad (D, \underline{x}) \mapsto f(D, \underline{x}) = \frac{\sqrt{\det D}}{\sqrt{(2\pi)^n}} \exp\left(-\frac{1}{2}\langle \underline{x}, D\underline{x} \rangle\right) . \quad (5)$$

For arbitrary point $D \in M_n^+$ the tangent space at D $T_D M_n^+$ can be identified by the vector space of the $n \times n$ real, symmetric matrices. For every point $D \in M_n^+$ and for every tangent vectors at D $X, Y \in T_D M_n^+$ the Riemannian metric is the following

$$g^{(\mathbf{F})}(D)(X, Y) = \int_{\mathbb{R}^n} \frac{1}{f(D, \underline{x})} \frac{\partial f(D, \underline{x})}{\partial X} \frac{\partial f(D, \underline{x})}{\partial Y} d\underline{x} , \quad (6)$$

where $\frac{\partial f(D, \underline{x})}{\partial X} = \frac{df(D+tX, \underline{x})}{dt} \Big|_{t=0}$.

The main geometrical quantities of the space $(M_n^+, g^{(\mathbf{F})})$ are computed. The Riemannian metric is expressed in terms of simple matrix operations (Theorem 2.23.) and I give a simple formula for this metric (Theorem 2.24.). The Levi–Civita connection, curvature tensor and scalar curvature are computed too (Equations 2.232–2.236).

2/b. The Fisher information defines Riemannian metric on the statistical model of discrete distributions and (special) n dimensional normal distributions. The geodesic equation is computed and solved and the geodesic distance in the case of the above mentioned Riemannian manifolds is given (Example 2.5. – 2.7.).

2/c. The set of the positive, selfadjoint $n \times n$ real (or complex) matrices of trace 1 is called real (or complex) state space. The elements of the real (or complex) state space are referred as real (or complex) states. (The states are sometimes called density matrices.) Let \mathcal{M}_n^+ be the interior of the state

space. This set \mathcal{M}_n^+ is the noncommutative generalization of the set of discrete distributions. The space \mathcal{M}_n^+ is a differentiable manifold and many relevant Riemannian metric can be defined on it. The statistically relevant Riemannian metrics are called monotone metrics. (The symbol $K^{(n)}$ denotes the monotone metric.) According to Petz theorem, every monotone metric can be described in terms of an operator monotone function $f :]0, \infty[\rightarrow \mathbb{R}$, with properties $f(x) = xf(x^{-1})$ and $f(1) = 1$ in a unique way. Such an operator monotone function f generates a metric: at the point $D \in \mathcal{M}_n^+$ and for tangent vectors $X, Y \in T_D\mathcal{M}_n^+$ the metric is the following

$$K_D^{(n),f}(X, Y) = \text{Tr} \left(X (R_{n,D}^{\frac{1}{2}} f(L_{n,D} R_{n,D}^{-1}) R_{n,D}^{\frac{1}{2}})^{-1} (Y) \right), \quad (7)$$

where $L_{n,D}$ and $R_{n,D}$ are the left and right multiplications. For example the monotone metric generated by the operator monotone function $f(x) = \frac{1}{4}(1 + \sqrt{x})^2$ is called Wigner–Yanase metric and denoted by $K_{\text{WY}}^{(n)}$.

The geodesic equation is computed and solved in the space $(\mathcal{M}_n^+, K_{\text{WY}}^{(n)})$ and the geodesic distance is given between states (Example 3.11.).

3. The differential geometrical quantities of the Riemannian manifold $(\mathcal{M}_n^+, K^{(n)})$ are analyzed since 1990. The scalar curvature was mentioned first by Petz [13], and he computed it for the manifold $(\mathcal{M}_2^+, K_{\text{KM}}^{(2)})$, where the metric $K_{\text{KM}}^{(2)}$ is the Kubo–Mori metric which is generated by the operator monotone function $f(x) = \frac{x-1}{\log x}$. The following result for the curvature was investigated by Petz and Sudár [15] in 1996, they computed the sectional curvature of the manifold \mathcal{M}_2^+ . The scalar curvature of the space $(\mathcal{M}_n^+, K_{\text{KM}}^{(n)})$ was computed by Michor, Petz and Andai [3] in the case of real states and by Dittmann [8] in the complex case for arbitrary monotone metric.

The scalar curvature for real and for complex state space for arbitrary monotone metrics is computed. It is shown that the geometrical structure of the state space is rather similar to the geometry of the n dimensional normal distribution (Part 4.1.).

4/a. The connection between the scalar curvature at a given state and statistical distinguishability and uncertainty in the neighborhood of the state is due to Petz [14]. Physically it is reasonable to believe that the more mixed states are less distinguishable. This means that the scalar curvature has a monotonicity property: if the state D_1 is more mixed than the state D_2 then the inequality $\text{Scal}(D_2) < \text{Scal}(D_1)$ should hold, where Scal denotes the scalar curvature. Petz conjecture is the following: the above mentioned monotonicity holds if the state space is endowed with the Kubo–Mori metric

[13]. Petz proved his conjecture in the case of 2×2 density matrices [13]. There are some numerical simulations for this conjecture, which confirm it. (In the classical case the scalar curvature is constant, so the conjecture holds.)

I consider the inequality in the Petz conjecture as the sum of five simpler inequalities. I give mathematical proof for some inequalities and the others are tested by computer programs [1] (Part 4.2.1.–4.2.3.). (I wrote numerical simulation programs for the Maple software.)

4/b. I prove that if the Petz conjecture holds in the space of complex density matrices, then it is true for real ones too (Theorem 4.8.).

5/a. The scalar curvature of the space of 2×2 density matrices is computed for arbitrary monotone metric using two different method (Theorem 4.11. and Example 4.1.). The Taylor expansion of the scalar curvature expression is given (Theorem 4.12.).

5/b. It is shown that every well-known monotone metrics generate monotone scalar curvature with respect the majorization on the space of 2×2 density matrices. Using the Taylor expansion of the scalar curvature function I give some monotone metrics on the space of 2×2 density matrices which generates non monotone scalar curvature (Theorem 4.14.) [2].

6. An explicit form is given for the scalar curvature on the space of 3×3 and 4×4 density matrices, when they are endowed by well known monotone metrics. Using numerical simulations I give example to such a monotone metric, which generates monotone scalar curvature with respect the majorization on the space of 2×2 density matrices, but it generates non monotone scalar curvature on the space of 3×3 density matrices. I give numerical evidences, that some monotone metrics generate monotone scalar curvature on the space of 4×4 density matrices too.

7. The differential geometrical quantities of the space of 2×2 density matrices are computed when it is endowed by well-known Riemannian metrics. The volume of the manifold is determined (Equations 4.295–4.297), the geodesic equation is given (Theorem 4.15.), the volume of the sphere which center is the most mixed state and the Taylor expansion of its volume is computed (Theorem 4.16.), and the Taylor expansion of the volume of a sphere with

arbitrary center is given when the manifold is endowed by well-known metrics (Equations 4.311–4.236). As an example, I illustrate such a spheres (Example 4.3.).

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