Jensen-Shannon divergence, Fisher information, and Wootters’ hypothesis

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Abstract

We discuss different statistical distances in probability space, with emphasis on the Jensen-Shannon divergence, vis-a-vis metrics in Hilbert space and their relationship with Fisher’s information measure. This study provides further reconfirmation of Wootters’ hypothesis concerning the possibility that statistical fluctuations in the outcomes of measurements be regarded (at least partly) as responsible for the Hilbert-space structure of quantum mechanics.

KEYWORDS: Fisher information, Jensen distance.

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I. INTRODUCTION

Wootters \cite{Wootters} has shown that nature defines the distance $D_W$ between two quantum states, say, $\psi_1$ and $\psi_2$, by counting the number of distinguishable intermediate states, which
establishes a link between statistics (distances in probability spaces, determined by the size of statistical fluctuations [1]) and geometry (metrics in Hilbert space) that has been considerably strengthened in [2]. The claim is made, however, that a proper understanding of this link needs still further elaboration [1], raising the interesting possibility that statistical fluctuations in the outcomes of measurements might be partly responsible for the Hilbert-space structure of quantum mechanics. An illuminating expansion of the work of [1] is provided in [2] and some footnotes can be found in [3]. Quite lucid, insightful, and also didactic mathematical treatments pertaining to the field of information geometry are those of Refs. [4–7] (see also references therein).

Obviously, the concept of distance between different rays in (the same) Hilbert space plays an important role in a variety of circumstances, like different preparations of the same system [1] or the geometric properties of the quantum evolution sub-manifold [8]. It is also relevant, for instance, in discussing squeezed coherent states, displaced number states, generalized coherent spin states, etc. [8], or for ascertaining the quality of approximate treatments [3]. One encounters it as well in connection with the detection of weak signals.

Inspired by the pioneer effort of Wootters [1], a set of well-known Hilbert space metrics were compared, in Ref. [3], to that underlying Wootters’ $D_W$. Let a quantum state $\psi_{\alpha}(x)$ be parameterized by $n$ real parameters collectively denoted by the symbol $\alpha$. A set of rays corresponding to the states with all possible $\alpha$-values constitutes an $n$-dimensional manifold $K$ of the Hilbert space $\mathcal{H}$. Set $\psi_1 = \psi_{\alpha}(x)$ and $\psi_2 = \psi_{\alpha+\Delta\alpha}(x)$. Expanding now $\psi_2$ in a $\Delta\alpha$-series, it was found in [3] that, up to second order in $\Delta\alpha$, several Hilbert space distances between $\psi_2$ and $\psi_1$ coincide with Wootters’ $D_W$, as does also the Kullback’s cross-entropy [9] between $|\psi_2|^2$ and $|\psi_1|^2$.

Here we will pursue the work of [3] i) by incorporating additional measures like the Jensen-Shannon divergence and, more importantly, ii) by providing still another interpretation to the role of fluctuations on which the work of Wootters’ originally focused attention.
II. FISHER’S INFORMATION MEASURE

An information measure can primarily be viewed as a quantity that characterizes a given probability distribution (PD) $\vec{P}$ [10,11]. Shannon’s logarithmic information measure [10]

$$S[\vec{P}] = -\sum_{j=1}^{N} p_j \ln(p_j),$$  

(1)

is regarded as the measure of the uncertainty associated to probabilistic physical processes described by the probability distribution $\{p_j, j = 1, \cdots, N\}$ ($\vec{P} \equiv (p_1, p_2, \cdots, p_N)$ the probability vector in the probability space $\Omega \subset \mathcal{R}^N$). We will be concerned here mainly with another important information-theoretic measure: that of Fisher’s ($I$) [12,13], advanced by R. A. Fisher in the twenties.

$I$ has been the subject of much work lately (a detailed study can be found in references [12,13]). Let us consider a system that is specified by a physical parameter $\alpha$, while $x$ is a stochastic variable ($x \in \mathcal{R}^N$) and $P_\alpha(x)$ the probability density for $x$, which depends on the parameter $\alpha$. An observer makes a measurement of $x$ and has to best infer $\alpha$ from this measurement, calling the resulting estimate $\tilde{\alpha} = \tilde{\alpha}(x)$. One wonders how well $\alpha$ can be determined. Estimation theory [14] asserts that the best possible estimator $\tilde{\alpha}(x)$, after a very large number of $x$-samples is examined, suffers a mean-square error $e^2$ for $\alpha$ that obeys a relationship involving Fisher’s $I$, namely, $Ie^2 = 1$, where the Fisher information measure $I$ is of the form

$$I(\alpha) = \int dx P_\alpha(x) \left\{ \frac{\partial \ln P_\alpha(x)}{\partial \alpha} \right\}^2.$$  

(2)

This “best” estimator is called the efficient estimator. Any other estimator must have a larger mean-square error. The only proviso to the above result is that all estimators be unbiased, i.e., satisfy $\langle \tilde{\alpha}(x) \rangle = \alpha$. Thus, the inverse of Fisher’s information measure provides a lower bound for the mean-square error $e^2$ associated with the statistical inference of the parameter $\alpha$. No matter what estimator we use (as long as it is an unbiased estimator) we have $e^2 \geq 1/I$. This inequality is referred to as the Cramer-Rao bound [13].
III. THE JENSEN-SHANNON DIVERGENCE

We review now some other measures with which we will be concerned in the present work and were not taken into account in [3]. Let $\vec{P}(k) \in \Omega \subset \mathcal{R}^N$, with $k = 1, 2$, denote two different probability distributions for a particular set of $N$ accessible states. The components of the two probability vectors $\vec{P}(k)$ must satisfy the following two constraints: 
a) $\sum_{j=1}^{N} p_j^{(k)} = 1$ and 
b) $0 \leq p_j^{(k)} \leq 1 \forall j$. The set $\Omega$ defined by these constraints is the simplex $S_N$, which is a convex $(N-1)$-dimensional subset of $R^N$. A quite important, information-theoretical based divergence measure between $\vec{P}(1)$ and $\vec{P}(2)$ was originally introduced by Lin [15] that came afterwards to be called the Jensen-Shannon divergence (JSD) [16,17] that

- induces a true metric in $\Omega \subset \mathcal{R}^N$, being indeed the square of a metric [18], and

- is intimately related to the Kullback-Leibler relative entropy $K$ for two probability distributions $\vec{P}(1)$ and $\vec{P}(2)$, given by [9]

$$K[\vec{P}(1) | \vec{P}(2)] = \sum_j p_j^{(1)} \ln \left( \frac{p_j^{(1)}}{p_j^{(2)}} \right). \quad (3)$$

We first define

$$J_0[\vec{P}(1), \vec{P}(2)] = K \left[ \vec{P}(1) \left| \left( \frac{1}{2} \vec{P}(1) + \frac{1}{2} \vec{P}(2) \right) \right. \right], \quad (4)$$

and then the symmetric quantity

$$J_1[\vec{P}(1), \vec{P}(2)] = J_0[\vec{P}(1), \vec{P}(2)] + J_0[\vec{P}(2), \vec{P}(1)] \quad (5)$$

$$= 2 \left[ S \left( \frac{1}{2} \vec{P}(1) + \frac{1}{2} \vec{P}(2) \right) - S[\vec{P}(1)] - S[\vec{P}(2)] \right].$$

Let now $\pi_1$, $\pi_2 > 0$; $\pi_1 + \pi_2 = 1$ be the “weights” of, respectively, the probability distributions $\vec{P}(1)$, $\vec{P}(2)$. The JSD reads

$$J_{\pi_1, \pi_2}[\vec{P}(1), \vec{P}(2)] = S \left[ \pi_1 \vec{P}(1) + \pi_2 \vec{P}(2) \right] - \pi_1 S[\vec{P}(1)] - \pi_2 S[\vec{P}(2)] \quad (6)$$

which is a positive-definite quantity that vanishes iff $\vec{P}(1) = \vec{P}(2)$ almost everywhere [16,17]. In the particular case $\pi_1 = \pi_2 = 1/2$ the measure (6) is symmetric. Notice also that

$$J_{\frac{1}{2}, \frac{1}{2}}^\frac{1}{2} = \frac{1}{2} J_1.$$
Using the q-information measures it is possible to construct a q-Kullback-Leibler relative entropy for two probability distributions. In particular, from the Tsallis entropy the q-Kullback entropy reads

\[
K_q^T[\vec{P}(1)|\vec{P}(2)] = - \sum_j p_j^{(1)} \ln \left( \frac{p_j^{(1)}}{p_j^{(2)}} \right).
\]  

(7)

IV. PRESENT RESULTS

Suppose that a quantum state \(\psi(x)\) is parameterized, as stated in the Introduction, by a real parameter that we denote by \(\alpha\), and write for simplicity \(\psi_\alpha(x) \equiv \psi(\alpha)\). We consider two states that differ by a change \(\alpha \rightarrow \alpha + \Delta \alpha\) and expand the second one up to second order in \(\Delta \alpha\) [we set \(\Delta^2 \alpha = (\Delta \alpha)^2\)].

\[
|\psi(\alpha + d\Delta \alpha) > = |\psi(\alpha) > + \Delta \alpha \frac{d}{d\alpha} |\psi(\alpha) > + \frac{1}{2} \Delta^2 \alpha \frac{d^2}{d\alpha^2} |\psi(\alpha) > + ... \tag{8}
\]

We wish to compare these associated wave functions (say, \(\psi_1\) and \(\psi_2\), by recourse to different measures. To this end, and following Eq. (8), we expand \(\psi(\alpha + \Delta \alpha)\) up to second order and assume that both \(\psi(\alpha)\) and \(\psi(\alpha + \Delta \alpha)\) are properly normalized to unity. For the present purposes we set \(P_{(1)} = |\psi(\alpha)|^2\) and \(P_{(2)} = |\psi(\alpha + \Delta \alpha)|^2\). The symmetrized Kullback-Leibler relative entropy

\[
K_S = K[\vec{P}(1)|\vec{P}(2)] + K[\vec{P}(2)|\vec{P}(1)]
\]  

(9)

is given by

\[
K_S = \int dx |\psi(\alpha)|^2 \ln \left[ \frac{|\psi(\alpha)|^2}{|\psi(\alpha + \Delta \alpha)|^2} \right] + \int dx |\psi(\alpha + \Delta \alpha)|^2 \ln \left[ \frac{|\psi(\alpha + \Delta \alpha)|^2}{|\psi(\alpha)|^2} \right]
\]  

(10)

For simplicity’s sake we restrict ourselves to one dimensional problems (the essentials of our discourse can already be apprehended at this stage) where, for stationary cases, one always can assume, without loss of generality, that wave functions are real. Up to second order in \(\Delta^2 \alpha\) (\(\psi' = \partial \psi / \partial \alpha\))
\[
[\psi(\alpha + \Delta \alpha)]^2 = \psi^2 \left[1 + \Delta \alpha \frac{\partial \ln \psi}{\partial \alpha} + \Delta^2 \alpha \left[\frac{\psi''}{\psi} + \left(\frac{\psi'}{\psi}\right)^2\right]\right],
\] (11)
so that
\[
P_{(2)} = P_{(1)} \left[1 + \Delta \alpha \frac{\partial \ln P_{(1)}}{\partial \alpha} + \frac{\Delta^2 \alpha P''_{(1)}}{2} + \ldots\right],
\] (12)
and we recast the Kullback-Leibler measure in the fashion
\[
K_S = -\int dx P_{(1)} \ln \left[1 + \Delta \alpha \frac{\partial \ln P_{(1)}}{\partial \alpha} + \frac{\Delta^2 \alpha P''_{(1)}}{2} \right]
\]
\[
+ \int dx P_{(1)} \left[1 + \Delta \alpha \frac{\partial \ln P_{(1)}}{\partial \alpha} + \frac{\Delta^2 \alpha P''_{(1)}}{2} \right]
\ln \left[1 + \Delta \alpha \frac{\partial \ln P_{(1)}}{\partial \alpha} + \frac{\Delta^2 \alpha P''_{(1)}}{2} \right].\] (13)

We will appeal to an expansion of \(\ln(1+y)\) up to first order in \(y\). Remember that both \(\psi(\alpha)\) and \(\psi(\alpha + \Delta \alpha)\) are properly normalized, which implies
\[
\Delta \alpha \int dx P_{(1)} \frac{\partial \ln P_{(1)}}{\partial \alpha} = 0,
\] (14)
and
\[
(\Delta^2 \alpha/2) \int dx P''_{(1)} = 0,
\] (15)
so that one obtains
\[
K_S = \Delta^2 \alpha \int dx P_{(1)} \left(\frac{\partial \ln P_{(1)}}{\partial \alpha}\right)^2 = \Delta^2 \alpha I(\alpha),
\] (16)
where \(I(\alpha)\) is the Fisher information measure defined in (2). This relation is to be expected on information-theoretic grounds [13], but, within the present context, it was not discussed neither in [3] nor in [1], so we wish to place strong emphasis on (16). Notice also that the Kullback-Leibler measure is stable against first order changes in \(\Delta \alpha\) [3].

Let us tackle now a subject that is new for the present scenario: the Jensen-Shannon divergence (4). Up to the second order in \(\Delta \alpha\) one has: i) for \(J_0\)
\[
J_0 \left[ P_{(1)}, P_{(2)} \right] = \frac{1}{8} \Delta^2 \alpha \int dx P_{(1)} \left(\frac{\partial \ln P_{(1)}}{\partial \alpha}\right)^2 = \frac{1}{8} \Delta^2 \alpha I(\alpha),
\] (17)
ii) for the symmetric $J_1$ of (5)

$$J_1[P_1, P_2] = \frac{1}{4} \Delta^2 \alpha \int dx P_1 \left( \frac{\partial \ln P_1}{\partial \alpha} \right)^2 = \frac{1}{4} \Delta^2 \alpha I(\alpha), \quad (18)$$

and iii) for the quantity defined in (6)

$$J^{\pi_1, \pi_2}[P_1, P_2] = \frac{\pi_1 \pi_2}{2} \Delta^2 \alpha \int dx P_1 \left( \frac{\partial \ln P_1}{\partial \alpha} \right)^2 = \frac{\pi_1 \pi_2}{2} \Delta^2 \alpha I(\alpha), \quad (19)$$

i.e., all the Jensen-Shannon divergences (17), (18), and (19), together with the Kullback-Leibler measure (16), are proportional to $I$, our main result thusfar. Now, it was shown in [3] that the Euclidean distance between neighboring states can be evaluated as

$$dS^2_E = \int dx \left[ \psi(\alpha + \Delta \alpha) - \psi(\alpha) \right]^2 = \Delta^2 \alpha \int dx \left| \frac{\partial \psi}{\partial \alpha} \right|^2,$$

so that it easily follows that, up to second order in $\Delta \alpha$, this distance is also proportional to $I$, that is well known to be a measure of the gradient of the probability-amplitude [13]

$$dS^2_E = \frac{1}{4} \Delta^2 \alpha I(\alpha), \quad (21)$$

which in the present context can be regarded as a new result. Additionally, by recourse to the comparison between $\psi(\alpha)$ and $\psi(\alpha + \Delta \alpha)$, we can relate the Euclidean distance with the Wootters one $D_W$. Using the following result from [3]

$$dS^2_E = 2(1 - <\psi(\alpha)|\psi(\alpha + \Delta \alpha)>) = 2(1 - \cos \gamma), \quad (22)$$

where $\gamma$ is a small angle, and now expanding $\cos \gamma$ up to order $\gamma^2$ one obtains

$$dS^2_E \cong \gamma^2 = [\arccos(<\psi(\alpha)|\psi(\alpha + \Delta \alpha)>)^2 = dS^2_W = D_W \quad (23)$$

where $D_W \equiv dS^2_W$ is the Wootters distance [3], so that Eq.(21) is tantamount to

$$dS^2_W = \frac{1}{4} \Delta^2 \alpha I(\alpha), \quad (24)$$

which can also regarded as a new result within the current context. We pass now to the celebrated Fubini-Study metric [19,20]. Considering neighboring states we have [3]
\[ dS_\tilde{K}^2 = 1 - |\langle \psi(\alpha) | \psi(\alpha + \Delta \alpha) \rangle |^2, \] (25)

which, after our by now familiar expansion up to second order yields

\[ dS_\tilde{K}^2 = \Delta^2 \alpha \int dx \left| \frac{\partial \psi}{\partial \alpha} \right|^2 = \frac{1}{4} \Delta^2 \alpha I(\alpha). \] (26)

Again, the Euclidean distance, and also the Wootters’ and Fubini-Study ones, are stable against first order changes in \( \Delta \alpha \) and all of them coincide, up order \( \Delta^2 \alpha \), with the \( J_1 \) Jensen-Shannon divergence, \textit{still another new result}. All these distances are proportional to the concomitant Fisher measure.

\textbf{V. DISCUSSION}

Let us examine a bit more closely the problem of estimating a single parameter (\( \alpha \)) of a system or phenomenon from knowledge of some measurements of the variable \( x \) [13]. Consider that we have at our disposal \( N \) data values of this variable \( x_1, \ldots, x_N \equiv x \). The system or phenomenon is governed by the conditional probability law (likelihood law) \( f(x|\alpha) \equiv f_\alpha(x) \). The data obey

\[ x = \alpha + y; \quad (y \ \text{added noise values,}), \] (27)

with \( y \) assumed to be intrinsic to the parameter \( \alpha \) under measurement. As an example, \( \alpha \) could be a particle’s position and \( y \) its concomitant fluctuations. The system consisting of quantities \( \alpha, y, x \) is a closed one [13]. The data are used in an estimation principle to form an estimate \( \tilde{\alpha} \) of \( \alpha \) which is a function of all the data (say, \( \sum_i^N x_i / N \)), and one assumes that the overall measurement procedure is “smart” in the sense that \( \tilde{\alpha} \) is on average a better estimate of \( \alpha \) than any of the data observables [13]. We see then that, on account of the Cramer-Rao bound \( I \) carries information with regards to intrinsic uncertainties, which, quantum mechanically, correspond to intrinsic fluctuations [13]. It is \textit{in this light that we have to regard the results of the preceding Section.}

The metric structure of the manifold \( K \) is completely expressed by the uncertainties and correlations of Hermitian operators generating various evolutions of a given quantum state.
[8] which are neatly captured by the Fubini metric, as has been demonstrated by using squeezed states [21]. But this metric does coincide, up to second order, with all the others considered here, and with $D_W$ in particular, that gave rise to the Wootters’ suggestion mentioned in the Introduction: *statistical fluctuations in the outcomes of measurements might be partly responsible for the Hilbert-space structure of quantum mechanics*. This view is now considerably strengthened in discovering that all distances (here considered) between quantum neighboring states, whether of statistical or Hilbert’s metric origin, are proportional to Fisher’s measure, up to second order approximation. Now,

- since $I$ captures, as pointed out above, the *essentially fluctuating nature* of the variables $x$ on which the state $\psi_\alpha(x)$ depends, and
- distances between neighboring states are proportional to $I$, it follows that
- Wootters’ viewpoint receives yet further (independent) reconfirmation.

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