Bayesian Thermostatistical Analyses of Two-Level Complex and Quaternionic Quantum Systems

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(April 1, 2022)

The three and five-dimensional convex sets of two-level complex and quaternionic quantum systems are studied in the Bayesian thermostatistical framework introduced by Lavenda. Associated with a given parameterization of each such set is a quantum Fisher (Helstrom) information matrix. The square root of its determinant — adopting an ansatz of Harold Jeffreys — provides a reparameterization-invariant prior measure over the set. Both such measures can be properly normalized and their univariate marginal probability distributions — which serve as structure functions — obtained. Gibbs (posterior) probability distributions can then be found, using Poisson’s integral representation of the modified spherical Bessel functions. The square roots of the (classical) Fisher information of these Gibbs distributions yield (unnormalized) priors over the inverse temperature parameters.

PACS Numbers 05.30.Ch, 03.65.-w, 02.50.-r

In this letter, we apply the Bayesian thermostatistical framework of Lavenda [1–3] to the two-level quantum systems, both complex and quaternionic [4] in nature. A two-level quaternionic system can be represented by a 2 \times 2 density matrix

\[ \rho = \frac{1}{2} \begin{pmatrix} 1 + z & x - iy - ju - kv \\ x + iy + ju + kv & 1 - z \end{pmatrix}, \]

where \( i^2 = j^2 = k^2 = -1, \quad ij = -ji = k, \quad jk = -kj = i, \quad ki = -ik = j \). Setting \( u = v = 0 \), we obtain the familiar (Pauli matrix) representation of the two-level complex systems [5, sec. 4.2], in which the points \((x, y, z)\) lie within the unit ball \(x^2 + y^2 + z^2 < 1\).

In the complex case \((u = v = 0)\), one can — using the concept of a symmetrized logarithmic derivative [6–11] — associate with the given parameterization, the quantum Fisher information matrix,

\[ \frac{1}{1 - x^2 - y^2 - z^2} \begin{pmatrix} 1 - y^2 - z^2 & xy & xz \\ xy & 1 - x^2 - z^2 & yz \\ xz & yz & 1 - x^2 - y^2 \end{pmatrix}. \]

In the quaternionic instance, employing the relations between the Pauli matrices and the quaternions [4, p. 495] [12, p. 197] to generate a complex 4 \times 4 complex density matrix and then finding the corresponding symmetrized logarithmic derivatives [11] — one has

\[ \frac{1}{1 - u^2 - v^2 - x^2 - y^2 - z^2} \begin{pmatrix} g(u) & uv & ux & uy & uz \\ uv & g(v) & vx & vy & vz \\ ux & vx & g(x) & xy & xz \\ uy & vy & xy & g(y) & yz \\ uz & vz & xz & yz & g(z) \end{pmatrix}, \]

where \( g(u) \) denotes \( 1 - u^2 - x^2 - y^2 - z^2 \) \ldots \) (The inverses of (2) and (3) provide — by the Cramér-Rao inequality — lower bounds [in the sense of negative definiteness] on the covariance matrices of the parameters [3]). The determinants of (2) and (3) are, respectively,

\[ \frac{1}{1 - x^2 - y^2 - z^2} \]

and

\[ \frac{1}{1 - u^2 - v^2 - x^2 - y^2 - z^2}. \]

(These are inversely proportional to the determinants obtained from (1) itself.)
In the classical/nonquantum situation — in which probability distributions rather than density matrices are studied — Harold Jeffreys proposed that one employ the square root of the determinant of a Fisher information matrix as a (reparameterization-invariant) prior measure (volume element) over a family (Riemannian manifold) of probability distributions \[13–15\]. Adopting this ansatz to the quantum mechanical case, one can — normalizing the square roots of (4) and (5) over the three and five-dimensional unit balls — derive the prior probability distributions,

\[
\frac{1}{\pi^2(1 - x^2 - y^2 - z^2)^{1/2}}, \quad (x^2 + y^2 + z^2 \leq 1)
\]  

and

\[
\frac{2}{\pi^3(1 - u^2 - v^2 - x^2 - y^2 - z^2)^{1/2}}, \quad (u^2 + v^2 + x^2 + y^2 + z^2 \leq 1)
\]  

The three bivariate marginal probability distributions of (6) are uniform over unit disks, while the five quadrivariate marginal probability distributions of (7) are uniform over unit balls in four-space. Further integrating over all but the last coordinate, one arrives at a univariate probability distribution, having the form, in the complex case,

\[
\frac{2(1 - z^2)^{1/2}}{\pi}, \quad (-1 \leq z \leq 1)
\]

and, in the quaternionic instance,

\[
\frac{8(1 - z^2)^{3/2}}{3\pi}, \quad (-1 \leq z \leq 1).
\]

We consider (8) and (9) to be (normalized) structure functions in the sense of Lavenda \[1–3\]. Since (8) and (9) are proportional to expressions of the type,

\[
(1 - z^2)^{n-1/2}, \quad (n = 1, 2)
\]

one can employ Poisson’s integral representation of the modified spherical Bessel functions (cylinder functions of half integral order) \[16\],

\[
I_n(\beta) = \left(\frac{\beta}{\pi}\right)^n \frac{\sqrt{\pi \Gamma(n + \frac{1}{2})}}{\sqrt{\pi \Gamma(n + \frac{3}{2})}} \int_{-1}^{1} \exp(-\beta z)(1 - z^2)^{n-1/2}dz
\]

(11)

to introduce thermodynamic considerations \[17–19\]. One then has (properly normalized) Gibbs distributions of the form,

\[
\frac{\exp(-\beta z)(\frac{\beta}{\pi})^n (1 - z^2)^{n-1/2}}{I_n(\beta) \sqrt{\pi \Gamma(n + \frac{3}{2})}},
\]

(12)

where \(\beta\) serves as the inverse temperature parameter. For \(\beta = -1\), Fig. 1 shows these distributions for \(n = 1\) (complex) and \(n = 2\) (quaternionic), the latter curve having the higher peak.

FIG. 1. Gibbs distributions (12) for \(\beta = -1\). The higher-peaked curve corresponds to the quaternionic \((n = 2)\) case.
Fig. 2 displays the analogous results for $\beta = 5$, with the curve for the complex case now having the higher peak.

![Probability density graph](image)

FIG. 2. Gibbs distributions (12) for $\beta = 5$. The lower-peaked curve corresponds to the quaternionic ($n = 2$) case.

In Fig. 3 and 4 are shown, respectively, the expected value of $z$ ($< z >$) and the variance about $< z >$ as a function of $\beta$, with the quaternionic curves being the flatter ones in the two graphs.

![Expected value graph](image)

FIG. 3. Expected value of $z$ as a function of $\beta$. The quaternionic ($n = 2$) curve is the flatter one.
FIG. 4. The variance about the expected value of \( z \) as a function of \( \beta \). The quaternionic \((n = 2)\) curve is the flatter one.

In Fig. 5 are displayed the relative entropies of the Gibbs distributions (12) with respect to the uniform distribution \((\frac{1}{2})\) over \( z \in [-1,1] \), with the quaternionic curve having the greater minimum.

FIG. 5. Relative entropy of Gibbs distributions with respect to a uniform distribution. The quaternionic \((n = 2)\) curve is the one having a greater minimum.

Since for \( n = 1, 2 \), in particular, the Gibbs distributions (12) form two families of probability distributions, each parameterized by \( \beta \), one can find the (classical) Fisher information associated with them [1,2,15]. This is accomplished by computing the negatives of the expected values (relative to (12)) of the second derivatives of the logarithms of (12) \((n = 1, 2)\) with respect to \( \beta \). The required integrations were performed numerically. The square roots of the obtained Fisher information statistics are exhibited in Fig. 6 for \( \beta \in [-10,10] \), with the quaternionic \((n = 2)\) case having the smaller maximum.
These serve as the Jeffrey’s (unnormalized) priors over the inverse temperature parameter (β), in the sense of Lavenda’s pioneering investigations [1–3]. (Fig. 6 was also reproducible, with MATHEMATICA, using exact/numerical methods, but only by taking the required integrations over \( z \in [-1, 1] \) — which themselves proved to be problematical — to be the results of integrations over \( z \in [0, 1] \) and the addition to them of the outcomes of substituting \(-β\) for \( β\) in them.)

For literature supplemental to [1, 2] pertaining to the topic of temperature fluctuations, see [20–28]. The quantum Fisher information metric [9] employed here to generate the structure (prior) functions (8) and (9) has been shown [10] to be simply proportional to the Bures metric — which extends to the mixed states, the Fubini-Study metric on the pure states of a quantum system.

ACKNOWLEDGMENTS

I would like to express appreciation to the Institute for Theoretical Physics for computational support in this research.

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