Metric-Dependent Probabilities that Two Qubits are Separable

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Abstract

In a previous study (*Quant. Info. Proc.* 1, 397 [2002]), we formulated a conjecture that arbitrarily coupled qubits — describable by 4×4 density matrices — are separable with an *a priori* probability of $\frac{8}{11\pi^2} \approx 0.0736881$. For this purpose, we employed the normalized volume element of the *Bures* (minimal monotone) metric as a probability distribution over the *fifteen-dimensional* convex set of 4×4 density matrices. Here, we provide further/independent (quasi-Monte Carlo numerical integration) evidence of a *stronger* nature (giving an estimate of 0.0736858 *vs.* 0.0737012 previously) for this conjecture. Additionally, employing a certain *ansatz*, we estimate the probabilities of separability based on certain other monotone metrics of interest. However, we find ourselves, at this point, unable to convincingly conjecture exact simple formulas for these new (smaller) probabilities.

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An arbitrary state of two quantum bits (qubits) is describable by a 4×4 density matrix — an Hermitian, nonnegative definite matrix having trace unity. The convex set of all such density matrices is 15-dimensional in nature [1, 2]. Endowing this set with the statistical distinguishability (SD) metric [3], we were able in [4] to address the question (first essentially raised in [5] and later studied further in [6, 7, 8]) of what proportion of the 15-dimensional convex set (now a Riemannian manifold) is separable (classically correlated) [9]. The Peres-Horodecki partial transposition criterion [10, 11] provides a convenient necessary *and* sufficient condition for testing for separability in the cases of qubit-qubit and qubit-qutrit pairs [12].

In [4] we had taken the probability of separability of two arbitrarily paired qubits to be the ratio of the SD volume (V_{SD}^s) occupied by the separable states to the SD volume (V_{SD}^{s+n}) occcupied by the totality of separable *and* nonseparable states. We utilized a conjecture (combining exact and numerical results) that

$$V_{SD}^{s+n} = \frac{\pi^8}{1680} \approx 5.64794, \tag{1}$$

the full veracity of which has since been formally established, within an impressively broad analytical framework [13, eq. (4.12)]. Then, on the basis of certain extended, advanced quasi-Monte Carlo computations (scrambled Halton sequences [14]), used for numerical integration in high-dimensional spaces, we had been led to further conjecture in [4] that

$$V_{SD}^s = \frac{\pi^6}{2310} \approx 0.416186. \tag{2}$$

(In an earlier study [8], a number of quite surprisingly simple *exact* results were obtained using *symbolic* integration, for certain specialized [low-dimensional] two-qubit scenarios — which had led us to entertain the possibility in [4] of an exact probability of separability in the full 15-dimensional setting.) For a scrambled Halton sequence consisting of 65 million points distributed over a 15-dimensional hypercube, we had obtained in [4] estimates of 5.64851 and .416302 of V_{SD}^{s+n} and V_{SD}^s, respectively.

Let us note that the interestingly-factorizable denominators in (1) and (2), that is, $1680 = 2^4 \cdot 3 \cdot 5 \cdot 7$ and $2310 = 2 \cdot 3 \cdot 5 \cdot 7 \cdot 11$ have been conjectured elsewhere [15, seq. A064377] (available on-line at www.research.att.com/ njas/sequences/Seis.html) to be the two *greatest* numbers (k) for which the sum of the *fourth* powers of the divisors of k exceeds the *fifth* power of the Euler totient function $\phi(k)$. ($\phi(k)$ is the number of positive integers — including 1 — less than k and relatively prime to k [16].)

The fundamental conjecture (2), of course, directly implied the further conjecture that the SD probability of separability is

$$P_{SD}^s = \frac{V_{SD}^s}{V_{SD}^{s+n}} = \frac{8}{11\pi^2} \approx 0.0736881. \tag{3}$$

Now, since the SD metric is identically *four* times the Bures (minimal monotone) metric [3], we have the immediate consequence that $P_{Bures}^s = P_{SD}^s$. (In regard to arbitrarily coupled qubit-*qutrit* pairs, we reached in [12], by similar methods, the conjecture that the corresponding probability of separability was the ratio ($\approx .00124706$) of $2^{20} \cdot 3^3 \cdot 5 \cdot 7$ to the product of π^3 and the seven consecutive prime numbers lying between 19 and 43.)

The Bures metric plays the role of the *minimal* monotone metric. The monotone metrics comprise an infinite (nondenumerable) class [17, 18, 19], generalizing the (classically *unique*) Fisher information metric [20]. The Bures metric has certainly been the most widely-studied member of this class [3, 13, 21, 22, 23, 24]. Two other prominent members are the *maximal* [25] and the *Kubo-Mori* (*KM*) [26, 27, 28] (also termed Bogoliubov-Kubo-Mori and Chentsov [29]) monotone metrics.

As to the maximal monotone metric, numerical, together with some analytical evidence, strongly indicate that V_{max}^{s+n} is infinite (unbounded) and that $P_{max}^s = 0$. (The supporting analytical evidence consists in the fact that for the three-dimensional convex set of 2×2 density matrices, parameterized by spherical coordinates $[r, \theta, \phi]$ in the "Bloch ball", the volume element of the maximal monotone metric is $r^2 \sin \theta (1 - r^2)^{-3/2}$, the integral of which *diverges* over the ball. Contrastingly, the volume element of the minimal monotone metric is $r^2 \sin \theta (1 - r^2)^{-1/2}$, the integral over the ball of which is *finite*, namely π^2.)

In this analysis, we will seek — analogously to our study of the SD/Bures metric in [4] — to determine $V_{\tilde{KM}}^s, V_{\tilde{KM}}^{s+n}$ and thus their ratio, P_{KM}^s. (A wiggly line over the acronym for a metric will denote here that we have multiplied that metric by 4, in order to facilitate comparisons with the results of our previous analysis [4], which had been presented primarily in terms of the SD, rather than the [proportional] Bures metric. The probabilities themselves — being ratios — are, of course, invariant under such a scaling, so the "wiggle" is irrelevant for them.) In particular, we first find compelling numerical evidence that

$$V_{\tilde{KM}}^{s+n} = 64 V_{SD}^s = \frac{4\pi^8}{105} \approx 361.468. \tag{4}$$

Then, using a scrambled *Faure* sequence [30] composed of 70 million points, rather than the

scrambled *Halton* sequences employed in [4], we obtain an estimate that

$$V^s_{K\tilde{M}} \approx 12.6822. \tag{5}$$

This leads us to the further estimates that

$$P^s_{KM} \approx .0350853, \tag{6}$$

and

$$\frac{P^s_{KM}}{P^s_{SD/Bures}} \approx .476147. \tag{7}$$

Critical to our analysis will be a certain *ansatz* that we have previously employed for similar purposes in [7]. Contained in the formula for the "Bures volume of the set of mixed quantum states" of Sommers and Życzkowski [13, eq. (3.18)], is the subexpression (following their notation)

$$Q_N = \Pi^{1...N}_{\nu<\mu} \frac{(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu}, \tag{8}$$

where ρ_μ, ρ_ν ($\mu, \nu = 1, \ldots, N$) denote the eigenvalues of an $N \times N$ density matrix. The term (8) can equivalently be rewritten using the "Morozova-Chentsov" function for the Bures metric [13, eq. (2.18)],

$$c_{Bures}(\rho_\mu, \rho_\nu) = \frac{2}{\rho_\nu + \rho_\mu} \tag{9}$$

as

$$Q_N = \Pi^{1...N}_{\nu<\mu} (\rho_\nu - \rho_\mu)^2 c_{Bures}(\rho_\mu, \rho_\nu)/2. \tag{10}$$

Our ansatz (working hypothesis) is that the replacement of c_{Bures} in the formulas for the Bures volume element by the particular Morozova-Chentsov function corresponding to a given monotone metric (g) will yield the volume element corresponding to g. We have been readily able to validate this for a number of instances in the case of the two-level quantum systems [$N = 2$], using the general formula for the monotone metrics over such systems of Petz and Sudär [17, eq. (3.17)].

We note here that the Morozova-Chentsov function for the Kubo-Mori metric is [13, eq. (2.18)]

$$c_{KM}(\rho_\mu, \rho_\nu) = \frac{\log \rho_\nu - \log \rho_\mu}{\rho_\nu - \rho_\mu}. \tag{11}$$

To proceed in this study, we first created a MATHEMATICA numerical integration program that succeeded to a high degree of accuracy in reproducing the formula [13, eq. (4.11)],

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TABLE I: Estimates based on the Bures and Kubo-Mori metrics, using a scrambled Faure sequence of 70 million points for numerical integration. In estimating P^s_{metric}, we use the *known* values of V^{s+n}_{metric} given by (1) and (2) — that is, 5.64794 and 361.468 — rather than the estimates of them reported in the table

metric	$V^{s+n}_{\tilde{metric}}$	$V^s_{\tilde{metric}}$	$P^s_{metric} = V^s/V^{s+n}$
Bures	5.64568	0.416172	0.0736858
Kubo-Mori	360.757	12.6822	0.0350853

$$C_N = \frac{2^{N^2-N}\Gamma(N^2/2)}{\pi^{N/2}\Gamma(1)\ldots\Gamma(N+1)} \tag{12}$$

for the Hall/Bures normalization constants [31, 32] for various N. (These constants form one of the two factors — along with the volume of the flag manifold [13, eqs. (3.22), (3.23)] — in determining the total Bures volume.) Then, in the MATHEMATICA program, we replaced the Morozova-Chentsov function for the Bures metric (9) in the product formula (10) by the one (11) for the Kubo-Mori function. For the cases, $N = 3, 4$ we found that the new numerical results were to several decimal places of accuracy (and in the case $N = 2$, exactly) equal to $2^{N(N-1)/2}$ times the comparable result for the Bures metric, given by (12). This immediately implies that the KM volumes of mixed states are also $2^{N(N-1)/2}$ times the corresponding Bures volumes (and the same for the $\tilde{KM}$ and SD volumes), since the remaining factors involved, that is, the volumes of the flag manifolds are common to both the Bures and KM cases (as well as to all the monotone metrics). Thus, we arrive at our assertion (4).

We then numerically integrated the $\tilde{KM}$ volume element over a fifteen-dimensional hypercube using points for evaluation in the hypercube determined by scrambled Faure sequences. (As in [4], the fifteen original variables parameterizing the 4×4 density matrices were first linearly transformed so as to all lie in the range [0,1].) These ("low discrepancy" [computationally intensive]) sequences are designed to give a close-to-*uniform* coverage of points over the hypercube, and thus hopefully yield accurate numerical integration results.

The results for the two monotone metrics considered so far are presented in Table I. The tabulated value of $P^s_{SD/Bures} \approx 0.0736858$ is closer to the conjectured value of $\frac{8}{11\pi^2} \approx$ 0.0736881 than the estimates (based on 65 million points of a scrambled Halton sequence)

obtained in [4], whether we scale there by the true value (1) of V_{SD}^{s+n} — which gives .0737087 — or scale by its estimated value there — which gives 0.0737012. (In a fully independent analysis based on 70 million points of a scrambled Halton sequence, we obtained estimates of $V_{\tilde{K}M}^{s+n}$ of 362.663, of $V_{\tilde{K}M}^{s}$ of 12.5809 and of P_{KM}^{s} of 0.034805.)

Associated with the minimal (Bures) monotone metric is the operator monotone function, $f_{Bures}(t) = (1+t)/2$, and with the maximal monotone metric, the operator monotone function, $f_{max}(t) = 2t/(1+t)$ [13, eq. (2.17)]. The *average* of these two functions, that is, $f_{average}(t) = (1 + 6t + t^2)/(4 + 4t)$, is also necessarily operator monotone [18, eq. (20)] and thus yields a monotone metric. Again employing our basic ansatz, we used the associated Morozova-Chentsov function (given by the general formula [17, p. 2667], $c(x,y) = 1/yf(x/y)$)

$$c_{average} = \frac{4(\rho_\mu + \rho_\nu)}{\rho_\mu^2 + 6\rho_\mu\rho_\nu + \rho_\nu^2}, \tag{13}$$

in the same quasi-Monte Carlo computations based on the scrambled Faure sequence composed of 70 million points. We obtained estimates of $V_{average}^{s+n} \approx 1.00888 \cdot 10^{35}$, $V_{average}^{s} \approx 2.825 \cdot 10^{22}$, so it appears that their ratio, $P_{average}^{s}$, is quite close to zero, if not exactly so (as we reasoned for the case of the maximal monotone metric itself).

Additionally, in an independent set of analyses (Table II), based on 160 million points of a scrambled Halton sequence, we sought to obtain estimates of the probability of separability of two arbitrarily coupled qubits based on three other monotone metrics of interest. These correspond to the operator monotone functions,

$$f_{WY}(t) = \frac{1}{4}(\sqrt{t} + 1)^2; \quad f_{GKS}(t) = t^{t/(t-1)}/e; \quad f_{NI}(t) = \frac{2(t-1)^2}{(1+t)\log(t)^2}. \tag{14}$$

The subscript WY denotes the Wigner-Yanase information metric [33, sec. 4] [34], the subscript GKS, the Grosse-Krattenthaler-Slater (or "quasi-Bures") metric (which yields the common asymptotic minimax and maximin redundancies for *universal* quantum coding [35, sec. IV.B] [36]), and the subscript NI, the "noninformative" metric (termed the Morozova-Chentsov metric in [37]).

On a concluding note, let us indicate that the seventy million points of the scrambled *Faure* sequence, central to our analyis, were computed in seven blocks of ten million each, on seven independent/non-communicating parallel processors (initialized with *different* random matrices). It is not totally clear to us at this stage, whether or not this is likely to be inferior to a (more time-demanding) computation on a *single* processor, or to the use of

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TABLE II: Estimates based on the Wigner-Yanase, Grosse-Krattenthaler-Slater and Noninformative monotone metrics, using a scrambled Halton sequence consisting of 160 million points. In estimating P^s_{metric}, as a ratio, we are compelled to use the estimated values of V^{s+n}_{metric}, unlike Table I, since their true values are not presently known

metric	$V^{s+n}_{\widetilde{metric}}$	$V^{s}_{\widetilde{metric}}$	$P^s_{metric} = V^s/V^{s+n}$
WY	446.615	2.1963	.0504375
GKS	166.906	.9938	.0610692
NI	3710.31	12.616	.0348745

seven processors all initialized with identical random matrices (cf. [38]). (In any case, it is certain that no such question needs to arise for the [fully deterministic] scrambled *Halton* sequences, also used here and in [4].) This matter is presently under our investigation. Nevertheless, in any case, we have achieved here rather impressive, improved convergence to our previously conjectured exact value (3) of $P^s_{SD/Bures}$.

Acknowledgments

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