Dimension-Independent Positive-Partial-Transpose Probability Ratios

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Abstract

We conduct quasi-Monte Carlo numerical integrations in two very high (80 and 79)-dimensional domains — the parameter spaces of rank-9 and rank-8 qutrit-qutrit \((9 \times 9)\) density matrices. We, then, estimate the ratio of the probability — in terms of the Hilbert-Schmidt metric — that a generic rank-9 density matrix has a positive partial transpose (PPT) to the probability that a generic rank-8 density matrix has a PPT (a precondition to separability/nonentanglement). Close examination of the numerical results generated — despite certain large fluctuations — indicates that the true ratio may, in fact, be 2. Our earlier investigation (eprint quant-ph/0410238) also yielded estimates close to 2 of the comparable ratios for qubit-qubit and qubit-qutrit pairs (the only two cases where the PPT condition fully implies separability). Therefore, it merits conjecturing (as Życzkowski was the first to do) that such Hilbert-Schmidt (rank-\(NM\)/rank-(\(NM-1\))) PPT probability ratios are 2 for all \(NM\)-dimensional quantum systems.

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Recent numerical analyses of ours \([1]\) have raised the possibility that there exists a certain quantum information-theoretic relation, independent of dimension \((NM)\), expressible in the form

\[
\Omega_{NM}^{HS} \equiv \frac{P_{NM}^{[HS,\text{rank}-(NM)]}}{P_{NM}^{[HS,\text{rank}-(NM-1)]}} = 2.
\]  

(1)

Here, HS denotes the Hilbert-Schmidt (HS) metric \([2, 3]\). \(\Omega_{NM}^{HS}\) is the ratio of the probability \(P_{NM}^{[HS,\text{rank}-(NM)]}\) that a full rank \(NM \times NM\) density matrix \((\rho)\) has a positive partial transpose (PPT) to the probability \(P_{NM}^{[HS,\text{rank}-(NM-1)]}\) of a density matrix of the same dimension but of rank one less \((NM-1)\) than full rank \((NM)\), having a PPT.

The partial transposition (PT) operation takes the \(N \times N\) blocks \((M^2\text{ in number})\) — or the \(M \times M\) blocks \((N^2\text{ in number})\) — of \(\rho\), and transposes them in place \([4, \text{ eq. (21)}]\). If none of the eigenvalues of the result is negative, as is necessarily the case with (the original, untransposed) \(\rho\) itself, by the properties of a density matrix, then the partial transposition is said to be positive. The Hilbert-Schmidt distance between two density matrices \((\rho_1\text{ and }\rho_2)\) is defined as the Hilbert-Schmidt (Frobenius) norm of their difference \([3, \text{ eq. (2.3)}]\),

\[
D_{HS}(\rho_1, \rho_2) = ||\rho_1 - \rho_2|| = \sqrt{\text{Tr}|(\rho_1 - \rho_2)^2|}.
\]  

(2)

The probabilities in the definition \([1]\) have a geometric interpretation. The numerator \(P_{NM}^{[HS,\text{rank}-(NM)]}\) is itself the ratio of the Hilbert-Schmidt \((N^2M^2 - 1)\)-dimensional volume of PPT states to the volume of all (PPT and non-PPT) states. The denominator \(P_{NM}^{[HS,\text{rank}-(NM-1)]}\) is the ratio of the \((N^2M^2 - 2)\)-dimensional “hyperarea” (bounding the volume) of rank-\((NM-1)\) PPT states to the hyperarea occupied by all rank-\((NM-1)\) states. (Exact formulas have recently become available for these total HS volumes and hyperareas \([3]\) (cf. \([5]\)), but not obviously for their PPT subsets — otherwise there would be no need for our numerical investigations here, as the true value of \([1]\) could, then, be simply directly computed.) \(\Omega_{NM}^{HS}\) can also be seen as the ratio of two hyperarea-to-volume ratios, one ratio based on all the states, and the other just on the PPT states.

We specifically studied in \([1]\) the cases \(N = 2, M = 2\) (qubit-qubit pairs) and \(N = 2, M = 3\) (qubit-qutrit pairs). Only in those two specific low-dimensional cases is having a PPT fully equivalent (by the Peres-Horodecki criterion \([4, 6]\)) to the property of separability (non-entanglement). For \(NM > 6\), the PPT condition is only necessary, but not sufficient for separability, and as Aubrun and Szarek have recently established becomes “weaker and weaker [in detecting separability] as the dimension increases” \([7]\). (Of course, it would be of
interest as well to study for $NM > 6$, ratios based on separability probabilities, rather than PPT probabilities, but that seems more difficult still (cf. [8, 9]). A state which has a PPT, and yet is not separable, exhibits “bound entanglement” [10] (cf. [11]).

Presented initially with only our qubit-qutrit analyses, Życzkowski proceeded to theorize — without yet a formal proof, however — that $\Omega_{NM}^{HS}$ is always equal to 2 for any $N = M$, and even possibly for $N \neq M$. (Perhaps we might also observe that when these conjectures were brought to the attention of S. Szarek, he commented that “the relationship can not be too hard [to prove] if true”.)

To be more specific, we had reported in [1, sec. VI C 2] — based on a quasi-Monte Carlo (Tezuka-Faure [12, 13]) numerical integration procedure, employing $4 \times 10^8$ sample points in 15- and 14-dimensional spaces (unit hypercubes) — an estimate in the qubit-qubit case of 2.00167 for $\Omega_4^{HS}$. For the qubit-qutrit analysis, $7 \times 10^9$ points in 35- and 34-dimensional hypercubes were utilized. An estimate of 2.0279 was obtained for $\Omega_6^{HS}$ [1, sec. VI C 1]. This was a (“pooled”) average of two estimates, based on two inequivalent ways of computing the PPT. When we generated the partial transpose by transposing in place the four $3 \times 3$ blocks of the corresponding $6 \times 6$ density matrices, our estimate was 1.99954, while when we transposed in place the nine $2 \times 2$ blocks, we obtained 2.05803 [1, last paragraph]. (Unfortunately, we lack any particular explanation for why one estimate should be so close to 2, while the other is relatively distant. It would appear that either some form of numerical instability is at work, or that the two types of partial transposition — surprisingly/puzzlingly — give rise to different (but close) Hilbert-Schmidt ratios. As illustrated in [1, sec. IV], a $6 \times 6$ density matrix can have a PPT under one such form of partial transposition, but not the other.)

Additionally, in [1, sec. VI C 3], we had reported the early stages of a qutrit-qutrit ($N = M = 3$) analysis. This was based on a similar procedural scheme with, at that stage, $126 \times 10^6$ Tezuka-Faure 80- and 79-dimensional points having been already generated. (To perform the required 79-dimensional numerical integration, we merely extracted, an essentially arbitrary subset from the 80-dimensional set, rather than going to the considerably greater computational expense of generating a totally new set of Tezuka-Faure points ab initio.) We reported the achieving, at a late stage of the analysis, of a cross-ratio of 1.89125, which we thought was encouragingly close to 2, for such an extraordinarily-challenging high-dimensional numerical integration problem. But we also had commented there that this ratio seemed subject to large fluctuations [1, Fig. 14], and in fact had further indicated that at
our last point generated, the ratio had sunk to approximately 0.15.

We have since continued this same numerical integration process from $126 \times 10^6$ to $500 \times 10^6$ (systematically-generated “low discrepancy”) points, and now look at it in more detail than in [1]. (In our analysis, we also include companion results based on the cross-norm criterion [14] — rather than partial transposition — which added substantially to our computational burden. We will only briefly discuss these results, as no particular theory/conjectures have been advanced as pertains to them. The cross-norm was not included in our earlier qubit-qubit and qutrit-qutrit analyses [1], so we have little basis for developing possible relevant hypotheses.)

We recorded the results of the 80-dimensional qutrit-qutrit numerical integration, at intermediate stages, for 250 intervals, each based on $2 \times 10^6$ points. For the 54-th to 61-st such intervals, our cumulative estimates of the Hilbert-Schmidt cross-ratio were

$$\{1.85599, 1.85619, 1.85765, 1.85915, 1.85941, 1.88103, 1.89082, 1.89125\}.$$  \(3\)

(Note the monotonic increase in the direction of the conjectured exact value of 2, as more points are sampled.)

Then, at the 62-nd interval, the estimate sharply plummeted to 0.208052. Now, we found that if we discard/ignore this interval (large fluctuation), and, then, in the resulting 249-member sequence of revised estimates, discard the 67-th interval, where the estimate drops similarly from 1.89181 to 0.0198977, we get in the new 248-member sequence of re-revised cumulative estimates, a 17-long additional sequence,

$$\{1.89083, 1.89098, 1.89101, 1.89056, 1.89181, 1.89892, 1.9031, 1.95864, 
1.96107, 1.95866, 1.95938, 1.95924, 1.98872, 1.98913, 1.98842, 1.98853, 1.98835\}.$$  \(4\)

which immediately follows upon the 8-long sequence of near-2 estimates \(3\), which was extracted from the original unedited 250-member sequence. So, we have — after only the two discardings — a consecutive/uninterrupted sequence of length 25 (= 8 + 17), all lying in the range [1.85,2]. Immediately following the last (25-th) member of this sequence (1.98835), the estimate first jumps to 2.09132 and then precipitously falls to 0.0786266. In Fig. 1, we plot the cumulative estimates of $(\Omega_{9}^{HS} - 2)$ for the edited sequence (containing 78 intervals, each based on $2 \times 10^6$ points) that ends just before this jump to 2.09132.
FIG. 1: Cumulative estimates of \((\Omega_{HS}^{9} - 2)\) based upon the first 78 intervals, after the discardings of two intervals (marked by large fluctuations) from the original 250-long sequence.

We could continue to similarly study the remainder of the 248-member sequence, discarding large fluctuations as they occur (of course, there is the difficult question of precisely defining them). But, at this stage, it would seem that we have already — coupled with our earlier qubit-qubit and qubit-qutrit results [1] — made a *prima facie* case for the plausibility of the Życzkowski conjecture stated above, which calls for its further investigation.

It would have been particularly appealing if a rational scheme had been found for editing the data, with the result that the final member of the sequence was near to 2. (As it stands, the last/250-th member of the [unedited] sequence did give us an estimate of 18.764 for the Hilbert-Schmidt ratio.) Of course, one might continue to add points, *via* the quasi-Monte Carlo procedure, to the 500 \(\times\) 10^6 already generated, in the (ensured [15]) expectation that convergence would *eventually* occur.

For the same (75-th) interval for which the Hilbert-Schmidt cross-ratio is closest to 2 (that is 1.98913), we obtained for the corresponding cross-ratio \((\Omega_{Bures}^{9})\) based, alternatively, on the Bures metric, an estimate of 0.260831; for the “arithmetic-average” metric, 0.236706; for the Wigner-Yanase metric, 0.172202; for the GKS/quasi-Bures metric, 0.21092; and for (the numerically rather unstable) Kubo-Mori metric, 0.0116725. (Such [monotone metric [16]] ratios were all close to 2 in the qubit-qutrit analysis, and approximately 1.8 in the qubit-qubit study [1].)

For the ratios based on the cross-norm rather than the PPT criterion, for which there are currently no conjectures, the analogous estimates at the same (1.98913) interval were — for the monotone metrics — 0.151657 [Bures], 16.718 [Kubo-Mori], 0.579336 [arithmetic-
average], 0.771286 [Wigner-Yanase], 0.287065 [GKS/quasi-Bures] and for the non-monotone Hilbert-Schmidt metric 2, 0.226471. (The corresponding estimates at the termination of the entire unedited 250-long sequence were, in the same order, 0.101299, 16.4129, 0.489673, 0.645947, 0.207893 and 0.223288.) The analysis also indicated that the cross-norm criterion is much weaker than the PPT in distinguishing states that could possibly be separable. (In sampling points over the 79- and 80-dimensional unit hypercubes that served as the domains of integration, roughly twenty-five times more points [9×9 density matrices] passed the cross-norm test than the PPT test. None at all that passed the cross-norm test failed the PPT one.)

The critical reader may have observed that we have not subjected any of the results above to statistical testing — the use of confidence intervals etc. The Tezuka-Faure procedure 12, 13 we have employed is highly efficient in finding well-distributed (low discrepancy) points, but does not lend itself in any natural fashion to statistical testing (there are variants, though, that do 15, 17, 18), such as with the much less efficient (random number) Monte Carlo methods. (The convergence rate of quasi-Monte Carlo is of order \( n^{-1+p/\log n}^{-1/2} \), where \( n \) is the dimension of the problem and \( p \) is a positive number. This is a worst case result. Compared to the expected rate \( n^{-1/2} \) of Monte Carlo, it shows the superiority of quasi-Monte Carlo 19, 20.)

This lack of statistical testability was, to some extent, compensated for in our earlier qubit-qubit and qubit-qutrit analyses 1, by the availability of exact formulas 3 for the Hilbert-Schmidt and Bures volumes and hyperareas of the \( N \times N \) density matrices, against which we could compare our numerical results, and thus assess their accuracy. They easily came within 1% of the true formulas in those two instances.

It would be of interest, as well, to study (PPT/separability) probability ratios for \( NM \times NM \) density matrices of ranks less than \( NM \) and \( (NM-1) \) 1, sec. VI C 4] (cf. 21, 22, 23). We are also, presently, investigating issues of a similar nature to those analyzed above in the \( (NM = 8) \) case of three-qubit states 24, 25, 26.

If the basic conjectured relation 11 holds, then one can deduce, using the known HS total-area-to-total-volume ratio 3, eq. (6.5)], that the ratio of the \( (N^2M^2 - 1) \)-volume of PPT states to the \( (N^2M^2 - 2) \)-hyperarea of PPT states must, in general, be equal to

\[
\frac{2}{\sqrt{NM(NM-1)(N^2M^2 - 1)}}
\]

In 1, sec. VI D 2] this relation, coupled with our numerical integration results, was used to hypothesize certain simple exact (well-fitting)
values for the HS volumes and hyperareas $individually$ of the separable qubit-qubit and qubit-qutrit states. Then, one immediately has implied formulas for the probabilities $P_{NM}^{[HS,\text{rank} - NM]}$ and $P_{NM}^{[HS,\text{rank} - (NM - 1)]}$.

The quasi-Monte Carlo (Tezuka-Faure) numerical integrations conducted here and in [1] over the domains (unit hypercubes) of the $NM \times NM$ density matrices, were all greatly facilitated by the use of the corresponding $Euler$ $angle$ parameterizations [2].

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