Detecting and Quantifying Entanglement via Bayesian Updating

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We show how a straightforward Bayesian updating procedure allows one to detect and quantify entanglement from any finite set of measurement results. The measurements do not have to be tomographically complete, and may consist of POVMs rather than von Neumann measurements. One obtains a probability that one's state is entangled and an estimate of any desired entanglement measure, including their error bars. As an example we consider (tomographically incomplete) spin correlation measurements on both 2-qubit and 3-qubit states. As byproducts we obtain an estimate of the volume of entangled states vs. states that violate a given Bell inequality for both pure and mixed states, and an inequality that relates the expectation value of the Bell operator to the negativity.

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Entanglement: useful, but hard to generate, and even harder to detect. The most measurement-intense approach to the problem of experimentally detecting the presence of entanglement is to perform complete quantum-state tomography [1]. Even for just two qubits this implies a reconstruction of all 15 independent elements of the corresponding density matrix. Subsequently applying the positive partial transpose (PPT) criterion to the reconstructed matrix gives a conclusive answer about entanglement or separability of the state [2, 3].

From the practical point of view it is desirable to have an entanglement detection tool which is more economical than full state tomography but nevertheless is decisive. Already in the original work on PPT [2] it was noticed that one can always construct an observable $\mathcal{W}$ with non-negative expectation values for all separable states ρ_s and a negative expectation value for at least one entangled state ρ_e. In this way an experimentally detected violation of the inequality $\langle\mathcal{W}\rangle \geq 0$ is a sufficient condition for entanglement. The observable $\mathcal{W}$ is called an entanglement witness (EW). The advantage of using EWs for entanglement detection will be appreciated better for multi-partite systems with more than 2 qubits, because the number of tomographic measurements would grow exponentially for such systems. On the other hand, a given witness does not detect all entangled states.

EWs assume the validity of quantum mechanics, and also assume one knows what measurements one is actually performing. A valuable alternative to EW can be sought in using a violation of Bell-CHSH inequalities [4, 5] as a sufficient condition for entanglement. Because Bell inequalities are derived from classical probability theory without any reference to quantum mechanics, no assumption about what is being measured is necessary. This method is, therefore, safe in the sense of avoiding many pitfalls arising from unwarranted (hidden) assumptions about one's experiment [6].

Here we propose a new method for entanglement detection that is in principle able to detect any entangled state, and which automatically takes into account finite data as well as imperfect measurements. The method produces an estimate of the relative probabilities that entangled and separable states are consistent with a given finite set of data. Thus our method differs from those in Refs [7–9] which assume expectation values of EWs are known [corresponding effectively to an *infinite* data set] and try to find the *minimally*-entangled state consistent with those expectation values.

We use a numerical Bayesian updating method for one's probability distribution over density matrices. A similar method was recently discussed in Ref. [10] in the context of quantum-state tomography. In particular, whereas the reconstruction of a density matrix from experimental data is usually based on the maximum likelihood estimation, Ref.[10] discusses its drawbacks and proposes Bayesian updating in its stead as a superior method. Our aim, though, is not to give an estimate of the density matrix, but, more modestly, to give estimates of entanglement and entanglement-related quantities.

A brief outline of our approach is as follows, and more details are given below. First, we choose a random finite test set of density matrices. We calculate the amount of entanglement (in fact, the negativity [11] for bipartite states, and measures derived from the negativity for multipartite systems) for each state in the set. The *a priori* probability that our unknown experimentally generated state, which we denote by $\rho_?$, equals a state ρ in the set is chosen as $\mathrm{p}(\rho) = 1/N$, where N is the number of states in the set. Second, we assume some set of POVMs with elements $\{\Pi_i\}$ is measured. These POVMs can describe any (noisy) set of measurements one performs on the qubits. Third, for the acquired measurement record $d = \{d_1, \cdots, d_i\}$ consisting of the number of times outcome i was obtained, we calculate the quantum-mechanical probability $\mathrm{p}(d|\rho)$ that a given state ρ from the test set generates the measurements outcome d (which follows directly from $\mathrm{Tr}\rho\Pi_i$). Having at hand probabilities $\mathrm{p}(d|\rho)$ for all states ρ in the test set we are now able to calculate the *a priori* probability $\mathrm{p}(d) = \sum_\rho \mathrm{p}(d|\rho) \cdot \mathrm{p}(\rho)$ for the measurement record d to occur. Fourth, we calculate – using Bayes' rule – the probability $\mathrm{p}(\rho|d)$ to have the state ρ for the given measurement outcomes d for all states ρ: $\mathrm{p}(\rho|d) = \mathrm{p}(d|\rho) \cdot \mathrm{p}(\rho)/\mathrm{p}(d)$. The fifth and the last step consists of reassigning $\mathrm{p}(\rho) := \mathrm{p}(\rho|d)$

for all states ρ. (After which we could repeat steps 2-5 for a new set of measurements d.)

This gives us the *a posteriori* probability that the unknown state $\rho_?$ equals the state ρ from the test set. From $\mathrm{p}(\rho|d)$ we can calculate the probability p_e for the state $\rho_?$ to be entangled. We just sum the probabilities $\mathrm{p}(\rho|d)$ for all entangled states ρ_{ent} in the set i.e.

$$\mathrm{p_e}(\rho_?) = \sum_{\rho=\rho_{ent}} \mathrm{p}(\rho|d). \tag{1}$$

Furthermore, we can calculate probability distributions for any function of the density matrix, such as the negativity and purity. We thus infer expectation values such as

$$\overline{N(\rho_?)} = \sum_{\rho=\rho_{ent}} \mathrm{p}(\rho|d) N(\rho), \tag{2}$$

and

$$\overline{P(\rho_?)} = \sum_{\rho} \mathrm{p}(\rho|d) \mathrm{Tr}(\rho^2), \tag{3}$$

as well as standard deviations $\sigma_N = \sqrt{\overline{N^2} - \bar{N}^2}$ etc.

The meaning of our final probability distribution $\mathrm{p}(\rho|d)$ is as follows. If we were forced to give a *single* density matrix that best describes all data and that includes error bars, we would give the highly mixed state $\bar{\rho} = \int d\rho \mathrm{p}(\rho)\rho$, as explained in [10]. The purity and negativity of the state $\bar{\rho}$ are *not* equal (smaller than, and typically much smaller than) to the estimates $\bar{N}$ and $\bar{P}$ that we use here. The difference is this: if one were to perform more measurements that are tomographically complete, $\bar{N}$ is the expected negativity. $N(\bar{\rho})$, instead, would be the useful entanglement of a *single* copy available without performing more measurements. For most quantum information processing purposes (such as teleportation) one indeed needs more precise knowledge about the density matrix than just its entanglement. See Ref. [6] for more discussions on this issue.

The only problem standing in the way of a straightforward application of Bayesian updating is that a sufficiently dense set is too hard to handle numerically, since even for 2-qubit density matrices the parameter space is 15-dimensional. Instead we update the test set itself *dynamically*: after calculating the likelihood for the initial test set of states, a large fraction (the bottom 99% of test states ordered by likelihood) is eliminated and replaced by new states, chosen at random around the surviving test states, with an equal number of new states added to each surviving test state. We thus use all data multiple times to construct better test sets. The spread Δ in the parameters characterizing our states (see below) is chosen to decrease exponentially from $\Delta = 0.5$ down to its minimum value $\Delta_f = 1/\sqrt{N_m}$ with N_m the total number of correlation measurements. Thus we "zoom in" on states that fit the data better while avoiding any bias among the best states. Since the procedure is random, we repeat this multiple times, and refer to the number of repetitions as "the number of runs." The number of times we update the test set within one run we will denote by "the number of iterations."

We used a standard representation [12, 13] of a random two-qubit density matrix as $\rho = U\rho_0 U^\dagger$, where $U \in SU(4)$ is randomly chosen and ρ_0 is a random diagonal density matrix. We parametrized the random unitaries U in a numerically convenient way, as $U = \exp(\sum_k ir_k\lambda_k)$, where the λ_k are 15 properly normalized generators of the Lie algebra $su(4)$, and r_k are random angles uniformly distributed over the interval $[-\pi, \pi]$. The random diagonal matrix is chosen by the same method as used in Ref. [12]. For three qubits, we apply a similar method, with $U \in$ SU(8). Of course, this choice of parametrization [which determines our prior probability distribution] may be natural, but is nevertheless subjective [as every prior is in Bayesian methods], and one is free to choose a different metric. The *a posteriori* probability of entanglement p_e should be compared to the *a priori* probability of entanglement. With our parametrization a random sample of 3×10^7 states showed a fraction $(36.437 \pm 0.010)\%$ to be entangled *a priori* (as compared to $(36.8 \pm 0.2)\%$ obtained in [12]). (More statistics follow below.)

In the following we consider, as an example, spin measurements performed on each qubit (considered as a spin-1/2 system) in *two* arbitrary spatial directions that are orthogonal, and we denote the corresponding spin operators by A_1 and A_2 for the first qubit, B_1 and B_2 for the second qubit, etc. For N qubits this constitutes 2^N correlation measurements. Since this set of measurements turned out to just fall short of estimating entanglement reliably for both the 2-qubit and 3-qubit states we tested, we add *one* more correlation function, namely where we measure the remaining third spatial direction on all qubits. This makes the set of measurements tomographically complete for the reduced density matrix of each qubit, but not for the full 2- or 3-qubit state.

We note that, in the 2-qubit case, we can construct four Bell-CHSH operators from the measured correlations:

$$\begin{aligned}
\mathcal{B}_1 &:= A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2), \\
\mathcal{B}_2 &= A_1 \otimes (B_1 + B_2) - A_2 \otimes (B_1 - B_2), \\
\mathcal{B}_3 &= A_1 \otimes (B_1 - B_2) + A_2 \otimes (B_1 + B_2), \\
\mathcal{B}_4 &= A_1 \otimes (-B_1 + B_2) + A_2 \otimes (B_1 + B_2).
\end{aligned} \tag{4}$$

We then test 2-qubit states that may be entangled but that do *not* violate any of the four Bell inequalities that can be constructed from these four operators (of course, if one would violate a Bell inequality, that would obviously detect entanglement in any case).

Our numerical results are displayed in Figs.1–6. For Figs. 1 and 2, we used 120 runs of 30 iterations each with a test set size of $N = 25,000$. In order to generate the expected probabilities and thus simulate a measurement record, we chose the unknown state $\rho_?$ to be a Werner-like state [14], $\rho_? = (1-p_W)\mathbb{1}/4 + p_W|\psi_+\rangle\langle\psi_+|$, where $|\psi_+\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$ is a maximally entangled state. Applying the PPT criterion to the state $\rho_?$ shows that it is entangled when $p_W > 1/3$. On the other hand, $\rho_?$ violates a Bell inequality only for $p_W > 1/2$. To demonstrate our approach we chose the value of p_W for entangled states to be tested in the range $(1/3, 1/2)$–so that no Bell inequality can be violated–and for separable states just outside this region (see Figures 1 and 2 for more details). In

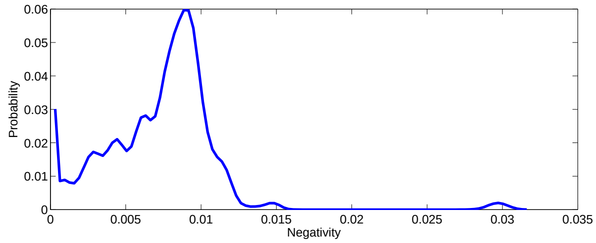

FIG. 1: Estimated probability distribution for the negativity, from $N_m = 5 \times 10,000$ simulated correlation measurements for an entangled Werner state with $p_W = 0.34$. From this probability distribution an estimate of the negativity $\bar{N}$ is obtained, as well as an estimate of the error bar: $\bar{N} = 0.0074 \pm 0.0038$, consistent with the negativity $N(\rho_?) = 0.01$ of the Werner state. The estimated probability of entanglement p_e is 97.0%. A similar simulation for a Werner state with $P_W = 0.33$, which is just not entangled, produced the result $\bar{N} = (2 \pm 6) \times 10^{-4}$, indicating no firm conclusion about entanglement can be reached in this border case.

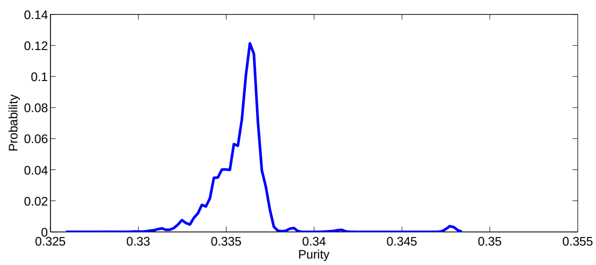

FIG. 2: Same as Fig. 1, but plotting the purity. The estimate is $\bar{P} = 0.3358 \pm 0.0017$ consistent with the purity of the Werner state $P = 0.3367$.

order to test the method itself, independent of fluctuations in the observed frequencies arising from finite statistics, we simply set the observed frequencies equal to the expected probabilities.

For Figs. 3 and 4 we used a different type of states containing less symmetry than the Werner states. We display just six runs but with much larger test sets. In this case, our method finds states that fit the data well, but with a smaller negativity than the state from which we derive the measurement record. This should not come as a surprise. Since we measure only five out of nine correlations, there is a four-dimensional manifold of states all fitting the data equally well. There is no reason that every such state possesses the same negativity, especially if our state lacks symmetry with respect to the measurements performed.

For the case of three qubits we choose the unknown state $\rho_?$ to be a three-qubit mixture of GHZ and W states,

$$\rho_? = p|GHZ\rangle\langle GHZ| + (1-p)|W\rangle\langle W|, \qquad (5)$$

with $p = \frac{3}{4}$. The measure of entanglement used is one advocated in [15],

$$N_{ABC} = (N_{A-BC} N_{B-AC} N_{C-AB})^{1/3}, \qquad (6)$$

in terms of the negativities of the three possible bipartite splits

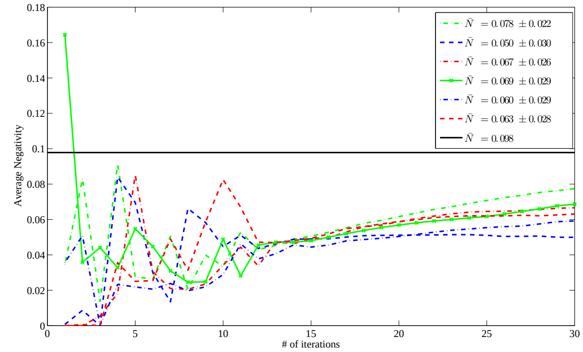

FIG. 3: Estimated negativity as a function of number of iterations for a randomly chosen state, for 6 runs: an equal mixture of states $(1, 2, 3, 4)/\sqrt{30}$ and $(4, 3, 2, -1)/\sqrt{30}$ [written in the standard basis], with negativity $N = 0.098$ and purity $P = 0.580$. The number of correlation measurements simulated is $5 \times 5,000$. The test set size is 4 million.

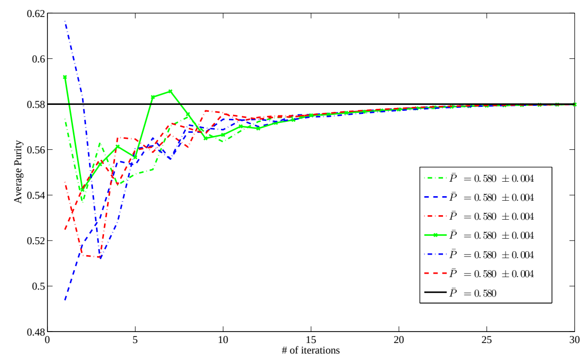

FIG. 4: Same as Fig. 3 but for the purity.

of a 3-qubit system. For this symmetric state our method finds the same negativity and purity, and 3 runs are displayed in Figs. 5 and 6.

We now return to Bell-CHSH inequalities for 2 qubits. The largest possible violation allowed by quantum mechanics is given by Cirel'son's bound $|\langle \mathcal{B}_i \rangle_{QM}| \leq 2\sqrt{2}$ [16]. On the other hand, it was recently shown by Uffink and Seevinck [17] that, in the special case that the measurements $A_{1,2}$ and $B_{1,2}$ correspond to spin measurements in orthogonal spatial directions, a significantly stronger inequality can be found for separable states. From that inequality one can derive a strengthened Bell inequality $|\langle \mathcal{B} \rangle| \leq \sqrt{2}$ (derived first by Roy in Ref. [18]). We will refer to this inequality as the Roy-Uffink-Seevinck (RUS) bound. We can generalize the RUS and Cirel'son's bounds for the same special choice of measurement operators,

$$|\langle \mathcal{B} \rangle_{\max}| \leq \sqrt{2}(1 + N(\rho)). \qquad (7)$$

The proof is straightforward and can be found in the first version of the present paper [19]. Eq. (7) contains both the RUS ($N \geq 0$) and Cirel'son's ($N \leq 1$) bounds. Moreover,

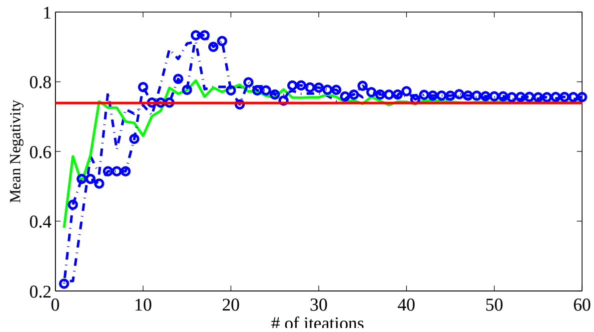

FIG. 5: Estimated negativity (see Eq. (6)) as a function of number of iterations for a mixture of three-qubit GHZ and W states with negativity $N_{ABC} = 0.740$ and purity $P = 0.630$. The number of correlation measurements simulated is $9 \times 5,000$. The test set size is 10^5.

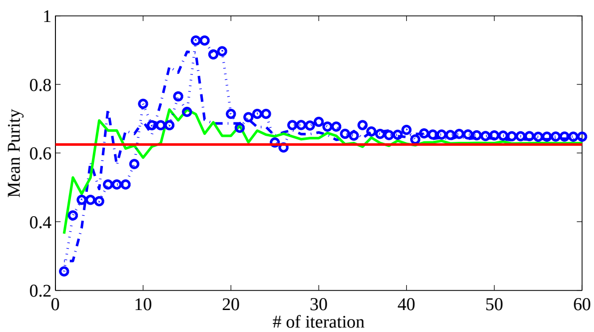

FIG. 6: Same as Fig. 5 but for the purity.

Eq. (7) provides a lower bound on the degree of entanglement in terms of negativity, if one violates the RUS bound. The bound complements the relations found in [21] between Bell inequalities and the concurrence and purity of mixed states.

Finally, from our numerical investigations we obtained the following *a priori* statistics for random mixed 2-qubit states: **(i)** Only a tiny fraction $(3.31 \pm 0.03) \times 10^{-4}$ violates at least one of the four Bell-CHSH inequalities that can be constructed from the operators (4). **(ii)** Only a small fraction $(1.244 \pm 0.003)\%$ violates at least one of the four RUS inequalities that can be constructed from the same operators (4).

For a similar set of *pure* random 2-qubit states (which are all entangled, except for a set of measure zero) we find: **(iii)** A fraction $(9.908 \pm 0.005)\%$ violates at least one of the four Bell-CHSH inequalities. **(iv)** A fraction $(46.627 \pm 0.010)\%$ violates at least one of the four RUS inequalities.

One should note that these statistics apply to a *fixed* set of correlation measurements involving spin measurements in 2 *fixed* orthogonal spatial directions. We also checked the case of a tomographically complete measurement, where one measures in 3 fixed spatial directions: from these data 36 Bell operators can be constructed. For mixed states the probability to violate at least one Bell inequality is still small, $(0.249 \pm 0.0008)\%$, and the probability to violate at least one RUS bound is $(5.690 \pm 0.004)\%$.

In conclusion, we have demonstrated a method to detect and quantify entanglement, using Bayesian updating for the probability distribution over density matrices. One obtains the probability that one's state is entangled as well as the value of any entanglement monotone, including estimates of statistical errors, of any type one needs. Quantifying entanglement is harder than merely verifying the presence of entanglement, but both objectives are achieved, as our Figures for sample cases of 2-qubit and 3-qubit states illustrate.

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[1] *Quantum State Estimation*, Series: Lecture Notes in Physics , Vol. 649 Paris, Matteo; Rehacek, Jaroslav (Eds.) 2004.
[2] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A **223**, 1 (1996).
[3] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).
[4] J. S. Bell, *Speakable and Unspeakable in Quantum Mechanics* (Cambridge University Press, Cambridge, 1987).
[5] J. Clauser, M. Horne, A. Shimony, and R. Holt, Phys. Rev. Lett. **23**, 880 (1969); J. F. Clauser, and M. Horne, Phys. Rev. D **10**, 526 (1974); J. F. Clauser and A. Shimony, Reports on Progress in Physics **41**, 1881, (1978).
[6] S. J. van Enk, N. Lütkenhaus, and H.J. Kimble, Phys. Rev. A **75**, 052318 (2007).
[7] K.M.R. Audenaert, M.B. Plenio, New J. Phys **8**, 266 (2006).
[8] J. Eisert, F.G.S.L. Brandão, K.M.R. Audenaert, New J. Phys **9**, 46 (2007).
[9] O. Gühne, M. Reimpell, R.F. Werner, Phys. Rev. Lett. **98**, 110502 (2007).
[10] R. Blume-Kohout, quant-ph/0611080.
[11] G. Vidal and R.F. Werner, Phys. Rev. A **65**, 032314 (2002).
[12] K. Zyczkowski *et al.*, Phys. Rev. A **58**, 883 (1998).
[13] T. Tilma, M. Byrd and E.C.G. Sudarshan, J. Phys. A **35**, 10445 (2002).
[14] R.F. Werner, Phys. Rev. A **40**, 4277 (1989).
[15] C. Sabin and G. Garcia-Alcaine, Eur. Phys. J. D **48**, 435 (2008).
[16] B.S. Cirel'son, Lett. Math. Phys. **4**, 93 (1980).
[17] J. Uffink and M. Seevinck, Phys. Lett. A **372**, 1205 (2008).
[18] S.M. Roy, Phys. Rev. Lett. **94**, 010402 (2005).
[19] Pavel Lougovski and S. J. van Enk, `arXiv:0806.4165`, version 1. The proof depends crucially on [20].
[20] F. Verstraete and H. Verschelde, Phys. Rev. A **66**, 022307 (2005).
[21] F. Verstraete and M.M. Wolf Phys. Rev. Lett. **89**, 170401 (2002).