Rank penalized estimation of a quantum system

Pierre Alquier[1], Cristina Butucea[2,4], Mohamed Hebiri[2], Katia Meziani[3], Tomoyuki Morimae[5,6]
[1] *University College Dublin, School of Mathematical Sciences, 528 James Joyce Library, Belfield, Dublin 4, Ireland*
[2] *LAMA, Université Marne-la-Vallée, 5, bd. Descartes, Champs-sur-Marne, 77454 Marne-la-Vallée Cedex 2*
[3] *CEREMADE, Université Paris Dauphine, Pl. du Maréchal De Lattre De Tassigny, 75775 Paris Cedex 16*
[4] *CREST, ENSAE, Timbre J-350, 3, av. Pierre Larousse, 92240 Malakoff*
[5] *Department of Physics, Imperial College London, SW7 2AZ, United Kingdom*
[6] *ASRLD Unit, Gunma University, 1-5-1 Tenjin-cho Kiryu-shi Gunma-ken, 376-0052, Japan*

We introduce a new method to reconstruct the density matrix ρ of a system of n-qubits and estimate its rank d from data obtained by quantum state tomography measurements repeated m times. The procedure consists in minimizing the risk of a linear estimator $\hat{\rho}$ of ρ penalized by given rank (from 1 to 2^n), where $\hat{\rho}$ is previously obtained by the moment method. We obtain simultaneously an estimator of the rank and the resulting density matrix associated to this rank. We establish an upper bound for the error of penalized estimator, evaluated with the Frobenius norm, which is of order $dn(4/3)^n/m$ and consistency for the estimator of the rank. The proposed methodology is computationaly efficient and is illustrated with some example states and real experimental data sets.

I. INTRODUCTION

The experimental study of quantum mechanical systems has made huge progress recently motivated by quantum information science. Producing and manipulating many-body quantum mechanical systems have been relatively easier over the last decade. One of the most essential goals in such experiments is to reconstruct quantum states via quantum state tomography (QST). The QST is an experimental process where the system is repeatedly measured with different elements of a positive operator valued measure (POVM).

Most popular methods for estimating the state from such data are: linear inversion [28], [24], maximum likelihood [4], [16], [21], [7], [29] and Bayesian inference [2], [3], [6] (we also refer the reader to [1, 8] and references therein). Recently, different approaches brought up-to-date statistical techniques in this field. The estimators are obtained via minimization of a penalized risk. The penalization will subject the estimator to constraints. In [18] the penalty is the Von Neumann entropy of the state, while [12], [13] use the $\mathbb{L}_1$ penalty, also known as the Lasso matrix estimator, under the assumption that the state to be estimated has low rank. These last papers assume that the number of measurements must be minimized in order to recover all the information that we need. The ideas of matrix completion is indeed, that, under the assumptions that the actual number of underlying parameters is small (which is the case under the low-rank assumption) only a fraction of all possible measurements will be sufficient to recover these parameters. The choice of the measurements is randomized and, under additional assumptions, the procedure will recover the underlying density matrix as well as with the full amount of measurements (the rates are within *log* factors slower than the rates when all measurements are performed).

In this paper, we suppose that a reasonable amount m (e.g. $m = 100$) of data is available from all possible measurements. We implement a method to recover the whole density matrix and estimate its rank from this huge amount of data. This problem was already considered by Guţă, Kypraios and Dryden [14] who propose a maximum likelihood estimator of the state. Our method is relatively easy to implement and computationally efficient. Its starting point is a linear estimator obtained by the moment method (also known as the inversion method), which is projected on the set of matrices with fixed, known rank. A data-driven procedure will help us select the optimal rank and minimize the estimators risk in Frobenius norm. We proceed by minimizing the risk of the linear estimator, penalized by the rank. When estimating the density matrix of a n-qubits system, our final procedure has the risk (squared Frobenius norm) bounded by $dn(4/3)^n/m$, where d between 1 and 2^n is the rank of the matrix.

The inversion method is known to be computationally easy but less convenient than constrained maximum likelihood estimators as it does not produce a density matrix as an output. We revisit the moment method in our setup and argue that we can still transform the output into a density matrix, with the result that the distance to the true state can only be decreased in the proper norm.

We shall indicate how to transform the linear estimator into a physical state with fixed, known rank. Finally, we shall select the estimator which fits best to the data in terms of a rank-penalized error. Additionally, the rank selected by this procedure is a consistent estimator of the true rank d of the density matrix.

We shall apply our procedure to the real data issued from experiments on systems of 4 to 8 ions. Trapped ion qubits are a promising candidate for building a quantum computer. An ion with a single electron in the valence shell is used. Two qubit states are encoded in two energy levels of the valence electrons, see [5], [14], [22].

The structure of the paper is as follows. Section 2 gives notation and setup of the problem. In Section 3 we present the moment method. We first change coordinates of the density matrix in the basis of Pauli matrices and vectorize the new matrix. We give properties of the linear operator which takes this vector of coefficients to the vector of probabilities $p(\mathbf{a}, \mathbf{r})$. These are the probabilities to get a certain outcome $\mathbf{r}$ from a given measurement indexed by $\mathbf{a}$ and that we actually estimate from data at our disposal. We prove the invertibility of the operator, i.e. identifiability of the model (the information we measure enables us to uniquely determine the underlying parameters). Section 4 is dedicated to the estimation procedure. The linear estimator will be obtained by inversion of the vector of estimated coefficients. We describe the rank-penalized estimator and study its error bounds. We study the numerical properties of our procedure on example states and apply them to experimental real-data in Section 5. The last section is dedicated to proofs.

II. BASIC NOTATION AND SETUP

We have a system of n qubits. This system is represented by a $2^n \times 2^n$ density matrix ρ, with coefficients in $\mathbb{C}$. This matrix is Hermitian $\rho^\dagger = \rho$, semidefinite positive $\rho \geq 0$ and has $\mathrm{Tr}(\rho) = 1$. The objective is to estimate ρ, from measurements of many independent systems, identically prepared in this state.

For each system, the experiment provides random data from separate measurements of Pauli matrices σ_x, σ_y, σ_z on each particle. The collection of measurements which are performed writes

$$\{\sigma_{\mathbf{a}} = \sigma_{a_1} \otimes \ldots \otimes \sigma_{a_n}, \quad \mathbf{a} \in \mathcal{E}^n = \{x, y, z\}^n\}, \qquad (1)$$

where $\mathbf{a} = (a_1, \ldots, a_n)$ is a vector taking values in $\mathcal{E}^n$ which identifies the experiment.

The outcome of the experiment will be a vector $\mathbf{r} \in \mathcal{R}^n = \{-1, 1\}^n$. It follows from the basic principles of quantum mechanics that the outcome of any experiment indexed by $\mathbf{a}$ is actually a random variable, say $R^{\mathbf{a}}$, and that its distribution is given by:

$$\forall \mathbf{r} \in \mathcal{R}^n, \mathbb{P}(R^{\mathbf{a}} = \mathbf{r}) = \mathrm{Tr}\left(\rho \cdot P_{r_1}^{a_1} \otimes \cdots \otimes P_{r_n}^{a_n}\right), \qquad (2)$$

where the matrices $P_{r_i}^{a_i}$ denote the projectors on the eigenvectors of σ_{a_i} associated to the eigenvalue r_i, for all i from 1 to n.

For the sake of simplicity, we introduce the notation

$$P_{\mathbf{r}}^{\mathbf{a}} := P_{r_1}^{a_1} \otimes \cdots \otimes P_{r_n}^{a_n}.$$

As a consequence we have the shorter writing for (2): $\mathbb{P}(R^{\mathbf{a}} = \mathbf{r}) = \mathrm{Tr}\left(\rho \cdot P_{\mathbf{r}}^{\mathbf{a}}\right)$.

The tomographic inversion method for reconstructing ρ is based on estimating probabilities $p(\mathbf{a}, \mathbf{r}) := \mathbb{P}(R^{\mathbf{a}} = \mathbf{r})$ by $\hat{p}(\mathbf{a}, \mathbf{r})$ from available data and solving the linear system of equations

$$\hat{p}(\mathbf{a}, \mathbf{r}) = \mathrm{Tr}\left(\hat{\rho} \cdot P_{\mathbf{r}}^{\mathbf{a}}\right). \qquad (3)$$

It is known in statistics as the method of moments.

We shall use in the sequel the following notation: $\|A\|_F^2 = \mathrm{Tr}(A^\dagger A)$ denotes the Frobenius norm and $\|A\| = \sup_{v \in \mathbb{R}^d, |v|_2 = 1} |Av|_2$ the operator sup-norm for any $d \times d$ Hermitian matrix A, $|v|_2$ is the Euclidean norm of the vector $v \in \mathbb{R}^d$.

In this paper, we give an explicit inversion formula for solving (2). Then, we apply the inversion procedure to equation (3) and this will provide us an unbiased estimator $\hat{\rho}$ of ρ. Finally, we project this estimator on the subspace of matrices of rank k (k between 1 and 2^n) and thus choose, without any a priori assumption, the estimator which best fits the data. This is done by minimizing the penalized risk

$$\|R - \hat{\rho}\|_F^2 + \nu \cdot \mathrm{rank}(R),$$

where the minimum is taken over all Hermitian, positive semidefinite matrices R. Note that the output is not a proper density matrix. Our last step will transform the output in a physical state. The previous optimization program has an explicit and easy to implement solution. The procedure will also estimate the rank of the matrix which best fits data. We actually follow here the rank-penalized estimation method proposed in the slightly different problems of matrix regression. This problem recently received a lot of attention in the statistical community [9, 17, 23, 26] and Chapter 9 in [20]. Here, we follow the computation in [9].

In order to give such explicit inversion formula we first change the coordinates of the matrix ρ into a vector $\vec{\rho} \in \mathbb{R}^{4n}$ on a convenient basis. The linear inversion also gives information about the quality of each estimator of the coordinates in $\vec{\rho}$. Thus we shall see that we have to perform all measurements $\sigma_{\mathbf{a}}$ in order to recover (some) information on each coordinate of $\vec{\rho}$. Also, some coordinates are estimated from several measurements and the accuracy of their estimators is thus better.

To our knowledge, this is the first time that rank penalized estimation of a quantum state is performed. Parallel work of Guţă *et al.* [14] addresses the same issue via the maximum likelihood procedure. Other adaptive methods include matrix completion for low-rank matrices [10, 12, 13, 19] and for matrices with small Von Neumann entropy [18].

III. IDENTIFIABILITY OF THE MODEL

Note the problem of state tomography with mutually unbiased bases, described in Section II, was considered in Refs. [11, 15]. In this section, we introduce some notation used throughout the paper, and remind some facts that were proved for example in [15] about the identifiability of the model.

A model is identifiable if, for different values of the underlying parameters, we get different likelihoods (probability distributions) of our sample data. This is a crucial property for establishing the most elementary convergence properties of any estimator.

The first step to explicit inversion formula is to express ρ in the n-qubit Pauli basis. In other words, let us put $\mathcal{M}^n = \{I, x, y, z\}^n$ and $\sigma_I = I$. For all $\mathbf{b} \in \mathcal{M}^n$, denote similarly to (1)

$$\{\sigma_{\mathbf{b}} = \sigma_{b_1} \otimes \ldots \otimes \sigma_{b_n}, \quad \mathbf{b} \in \mathcal{M}^n\}. \tag{4}$$

Then, we have the following decomposition:

$$\rho = \sum_{\mathbf{b} \in \mathcal{M}^n} \rho_{\mathbf{b}} \cdot \sigma_{\mathbf{b}}, \quad \text{with } \rho_{(I,\ldots,I)} = \frac{1}{2^n}.$$

We can plug this last equation into (2) to obtain, for $\mathbf{a} \in \mathcal{E}^n$ and $\mathbf{r} \in \mathcal{R}^n$,

$$\begin{aligned}
&\mathbb{P}(R^{\mathbf{a}} = \mathbf{r}) = \mathrm{Tr}\left(\rho \cdot P^{\mathbf{a}}_{\mathbf{r}}\right) \\
&= \mathrm{Tr}\left(\sum_{\mathbf{b} \in \mathcal{M}^n} \rho_{\mathbf{b}} \cdot \sigma_{\mathbf{b}} \cdot P^{\mathbf{a}}_{\mathbf{r}}\right) \\
&= \sum_{\mathbf{b} \in \mathcal{M}^n} \rho_{\mathbf{b}} \mathrm{Tr}\left((\sigma_{b_1} \otimes \cdots \otimes \sigma_{b_n}) \left(P^{a_1}_{r_1} \otimes \cdots \otimes P^{a_n}_{r_n}\right)\right) \\
&= \sum_{\mathbf{b} \in \mathcal{M}^n} \rho_{\mathbf{b}} \prod_{j=1}^{n} \mathrm{Tr}(\sigma_{b_j} P^{a_j}_{r_j}).
\end{aligned}$$

Finally, elementary computations lead to $\mathrm{Tr}(IP^t_s) = 1$ for any $s \in \{-1, 1\}$ and $t \in \{x, y, z\}$, while $\mathrm{Tr}(\sigma_t P^{t'}_s) = s\delta_{t,t'}$ for any $s \in \{-1, 1\}$, $(t, t') \in \{x, y, z\}^2$ and δ denotes the Kronecker symbol.

For any $\mathbf{b} \in \mathcal{M}^n$, we denote by $E_{\mathbf{b}} = \{j \in \{1, \ldots, n\} : b_j = I\}$. The above calculation leads to the following fact, which we will use later.

Fact 1 *For $\mathbf{a} \in \mathcal{E}^n$, and $\mathbf{r} \in \mathcal{R}^n$, we have*

$$\mathbb{P}(R^{\mathbf{a}} = \mathbf{r}) = \sum_{\mathbf{b} \in \mathcal{M}^n} \rho_{\mathbf{b}} \cdot \prod_{j \notin E_{\mathbf{b}}} r_j \, \mathbf{I}(a_j = b_j).$$

Let us consider, for example, $\mathbf{b} = (x, \ldots, x)$, then the associated set $E_{\mathbf{b}}$ is empty and $\mathbb{P}(R^{(x,\ldots,x)} = \mathbf{r})$ is the only probability depending on $\rho_{(x,\ldots,x)}$ among other coefficients. Therefore, only the measurement $(\sigma_x, \ldots, \sigma_x)$ will bring information on this coefficient. Whereas, if $\mathbf{b} = (I, I, x, \ldots, x)$, the set $E_{\mathbf{b}}$ contains 2 points. There are 3^2 measurements $\{(\sigma_x, ..., \sigma_x)$, ..., $(\sigma_z, \sigma_z, \sigma_x, ..., \sigma_x)\}$ that will bring partial information on $\rho_{\mathbf{b}}$. This means, that a coefficient $\rho_{\mathbf{b}}$ is estimated with higher accuracy as the size of the set $E_{\mathbf{b}}$ increases.

For the sake of shortness, let us put in vector form:

$$\begin{aligned}
\vec{\rho} &:= (\rho_{\mathbf{b}})_{\mathbf{b} \in \mathcal{M}^n} \\
\mathbf{p} &:= \left(p_{(\mathbf{r},\mathbf{a})}\right)_{(\mathbf{r},\mathbf{a}) \in (\mathcal{R}^n \times \mathcal{E}^n)} = (\mathbb{P}(R^{\mathbf{a}} = \mathbf{r}))_{(\mathbf{r},\mathbf{a}) \in (\mathcal{R}^n \times \mathcal{E}^n)}.
\end{aligned}$$

Our objective is to study the invertibility of the operator

$$\begin{aligned}
\mathbb{R}^{4^n} &\to \mathbb{R}^{6^n} \\
\vec{\rho} &\mapsto \mathbf{p}.
\end{aligned}$$

Thanks to Fact 1, this operator is linear. It can then be represented by a matrix

$\mathbf{P} = [P_{(\mathbf{r},\mathbf{a}),\mathbf{b}}]_{(\mathbf{r},\mathbf{a})\in(\mathcal{R}^n\times\mathcal{E}^n),\mathbf{b}\in\mathcal{M}^n}$, we will then have:

$$\forall(\mathbf{r},\mathbf{a}) \in (\mathcal{R}^n \times \mathcal{E}^n), \quad p_{(\mathbf{r},\mathbf{a})} = \sum_{\mathbf{b}\in\mathcal{M}^n} \rho_{\mathbf{b}} P_{(\mathbf{r},\mathbf{a}),\mathbf{b}} \tag{5}$$

and from Fact 1 we know that

$$P_{(\mathbf{r},\mathbf{a}),\mathbf{b}} = \prod_{j\notin E_{\mathbf{b}}} r_j \, \mathbf{I}(a_j = b_j).$$

We want to solve the linear equation $\mathbf{P}\vec{\rho} = \mathbf{p}$. Recall that $E_{\mathbf{b}}$ is the set of indices where the vector $\mathbf{b}$ has an I operator. Denote by $d(\mathbf{b})$ the cardinality of the set $E_{\mathbf{b}}$.

Proposition 2 *The matrix $\mathbf{P}^T\mathbf{P}$ is a diagonal matrix with non-zero coefficients given by*

$$(\mathbf{P}^T\mathbf{P})_{\mathbf{b},\mathbf{b}} = 3^{d(\mathbf{b})}\, 2^n.$$

As a consequence the operator is invertible, and the equation $\mathbf{P}\vec{\rho} = \mathbf{p}$ has a unique solution:

$$\vec{\rho} = (\mathbf{P}^T\mathbf{P})^{-1}\mathbf{P}^T\mathbf{p}.$$

In other words, we can reconstruct $\vec{\rho} = (\rho_{\mathbf{b}})_{\mathbf{b}\in\mathcal{M}^n}$ from $\mathbf{p}$, in the following way:

$$\rho_{\mathbf{b}} = \frac{1}{3^{d(\mathbf{b})}2^n} \sum_{(\mathbf{r},\mathbf{a})\in(\mathcal{R}^n\times\mathcal{E}^n)} p_{(\mathbf{r},\mathbf{a})}\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}.$$

This formula confirms the intuition that, the larger is $d(\mathbf{b})$, the more measurements $\sigma_{\mathbf{a}}$ will contribute to recover the coefficient $\rho_{\mathbf{b}}$. We expect higher accuracy for estimating $\rho_{\mathbf{b}}$ when $d(\mathbf{b})$ is large.

IV. ESTIMATION PROCEDURE AND ERROR BOUNDS

In practice, we do not observe $\mathbb{P}(R^{\mathbf{a}} = \mathbf{r})$ for any $\mathbf{a}$ and $\mathbf{r}$. For any $\mathbf{a}$, we have a set of m independent experiments, whose outcomes are denoted by $R^{\mathbf{a},i}$, $1 \le i \le m$. Our setup is that the $R^{\mathbf{a},i}$ are independent, identically distributed (i.i.d.) random variables, distributed as $R^{\mathbf{a}}$.

We then have a natural estimator for $p_{(\mathbf{r},\mathbf{a})} = \mathbb{P}(R^{\mathbf{a}} = \mathbf{r})$:

$$\hat{p}_{(\mathbf{r},\mathbf{a})} = \frac{1}{m}\sum_{i=1}^{m} \delta_{R^{\mathbf{a},i},\mathbf{r}}.$$

We can of course write $\hat{\mathbf{p}} = (\hat{p}_{(\mathbf{r},\mathbf{a})})_{(\mathbf{r},\mathbf{a})\in(\mathcal{R}^n\times\mathcal{E}^n)}$.

A. Linear estimator

We apply the inversion formula to the estimated vector $\hat{\mathbf{p}}$. Following Proposition 2 we can define:

$$\hat{\vec{\rho}} = (\mathbf{P}^T\mathbf{P})^{-1}\mathbf{P}^T\hat{\mathbf{p}}. \tag{6}$$

Put it differently:

$$\hat{\rho}_{\mathbf{b}} = \frac{1}{3^{d(\mathbf{b})}2^n} \sum_{(\mathbf{r},\mathbf{a})\in(\mathcal{R}^n\times\mathcal{E}^n)} \hat{p}_{(\mathbf{r},\mathbf{a})}\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}$$

and then, the linear estimator obtained by inversion, is

$$\hat{\rho} = \sum_{\mathbf{b}\in\mathcal{M}^n} \hat{\rho}_{\mathbf{b}}\sigma_{\mathbf{b}}. \tag{7}$$

The next result gives asymptotic properties of the estimator $\hat{\vec{\rho}}$ of $\vec{\rho}$.

Proposition 3 *The estimator $\hat{\vec{\rho}}$ of $\vec{\rho}$, defined in (6) has the following properties:*

1. *it is unbiased, that is $\mathbb{E}[\hat{\vec{\rho}}] = \vec{\rho}$;*
2. *it has variance bounded as follows*

$$Var(\hat{\rho}_{\mathbf{b}}) \le \frac{1}{3^{d(\mathbf{b})}4^n m};$$

3. *for any $\varepsilon > 0$,*

$$\mathbb{P}\left(\|\hat{\rho} - \rho\|^2 \ge 4\sqrt{2\left(\frac{4}{3}\right)^n \frac{n\log(2) - \log(\varepsilon)}{m}}\right) \le \varepsilon.$$

Note again that the accuracy for estimating $\rho_{\mathbf{b}}$ is higher when $d(\mathbf{b})$ is large. Indeed, in this case more measurements bring partial information on $\rho_{\mathbf{b}}$.

The concentration inequality gives a bound on the norm $|\hat{\vec{\rho}} - \vec{\rho}|_\infty$ which is valid with high probability. This quantity is related to $\|\hat{\rho} - \rho\|$ in a way that will be explained later on. The bound we obtain above depends on $\log(2^n)$, which is expected as $4^n - 1$ is the total number of parameters of a full rank system. This factor appears in the Hoeffding inequality that we use in order to prove this bound.

B. Rank penalized estimator

We investigate low-rank estimates of ρ defined in (7). From now on, we follow closely the results in [9] which were obtained for a matrix regression model, with some

differences as our model is different. Let us, for a positive real value ν study the estimator:

$$\hat{\rho}_\nu = \arg\min_R \left[\|R - \hat{\rho}\|_F^2 + \nu \cdot \mathrm{rank}(R) \right], \qquad (8)$$

where the minimum is taken over all Hermitian matrices R. In order to compute the solution of this optimization program, we may write it in a more convenient form since

$$\begin{aligned} &\min_R \left[\|R - \hat{\rho}\|_F^2 + \nu \cdot \mathrm{rank}(R) \right] \\ &= \min_k \min_{R:\mathrm{rank}(R)=k} \left[\|R - \hat{\rho}\|_F^2 + \nu \cdot k \right]. \qquad (9) \end{aligned}$$

An efficient algorithm is available to solve the minimization program (9) as a spectral-based decomposition algorithm provided in [25]. Let us denote by $\hat{R}_k$ the matrix such that $\|\hat{R}_k - \hat{\rho}\|_F^2 = \min_{R:\mathrm{rank}(R)=k} \left[\|R - \hat{\rho}\|_F^2 + \nu \cdot k \right]$. This is a projection of the linear estimator on the space of matrices with fixed (given) rank k. Our procedure selects automatically out of data the rank $\hat{k}$. We see in the sequel that the estimators $\hat{R}_{\hat{k}}$ and $\hat{\rho}_\nu$ actually coincide.

We study the statistical performance from a numerical point of view later on.

Theorem 4 *For any $\theta > 0$ put $c(\theta) = 1 + 2/\theta$. We have on the event $\{\nu \geq (1+\theta)\|\hat{\rho} - \rho\|^2\}$ that*

$$\|\hat{\rho}_\nu - \rho\|_F^2 \leq \min_k \left\{ c^2(\theta) \sum_{j>k} \lambda_j^2(\rho) + 2c(\theta)\nu k \right\},$$

where $\lambda_j(\rho)$ for $j = 1, \ldots, 2^n$ are the eigenvalues of ρ ordered decreasingly.

Note that, if $\mathrm{rank}(\rho) = d$, for some d between 1 and 2^n, then the previous inequality becomes

$$\|\hat{\rho}_\nu - \rho\|_F^2 \leq 2c(\theta)\nu d.$$

Let us study the choice of ν in Theorem 4 such that the probability of the event $\{\nu \geq (1+\theta)\|\hat{\rho} - \rho\|^2\}$ is small. By putting together the previous theorem and Proposition 3, we get the following result:

Corollary 5 *For any $\theta > 0$ put $c(\theta) = 1 + 2/\theta$ and for some small $\varepsilon > 0$ choose*

$$\nu(\theta, \varepsilon) = 32(1+\theta) \left(\frac{4}{3}\right)^n \frac{n\log(2) - \log(\varepsilon)}{m}$$

Then, we have

$$\|\hat{\rho}_{\nu(\theta,\varepsilon)} - \rho\|_F^2 \leq \min_k \left\{ c^2(\theta) \sum_{j>k} \lambda_j^2(\rho) + 2c(\theta)\nu k \right\},$$

with probability larger than $1 - \varepsilon$.

Again, if the true rank of the underlying system is d, we can write that, for any $\theta > 0$ and for some small $\varepsilon > 0$:

$$\|\hat{\rho}_\nu - \rho\|_F^2 \leq 64c(\theta)(1+\theta)d \left(\frac{4}{3}\right)^n \frac{n\log(2) - \log(\varepsilon)}{m},$$

with probability larger than $1 - \varepsilon$. If $\|\cdot\|_1$ denotes the trace norm of a matrix, we have $\|M\|_1 \leq 2^{\frac{n}{2}}\|M\|_F$ for any matrix M of size $2^n \times 2^n$. So, we deduce from the previous bound that

$$\|\hat{\rho}_\nu - \rho\|_1^2 \leq 64c(\theta)(1+\theta)d \left(\frac{8}{3}\right)^n \frac{n\log(2) - \log(\varepsilon)}{m}.$$

The next result will state properties of $\hat{k}$, the rank of the final estimator $\hat{\rho}_\nu$.

Corollary 6 *If there exists k such that $\lambda_k(\rho) > (1+\delta)\sqrt{\nu}$ and $\lambda_{k+1}(\rho) < (1-\delta)\sqrt{\nu}$ for some δ in $(0, 1]$, then*

$$\mathbb{P}(\hat{k} = k) \geq 1 - \mathbb{P}(\|\hat{\rho} - \rho\| \geq \delta\sqrt{\nu}).$$

From an asymptotic point of view, this corollary means that, if d is the rank of the underlying matrix ρ, then our procedure is consistent in finding the rank as the number m of data per measurement increases. Indeed, as $\sqrt{\nu}$ is an upper bound of the norm $\|\hat{\rho} - \rho\|$, it tends to 0 asymptotically and therefore the assumptions of the previous corollary will be checked for $k = d$. With a finite sample, we deduce from the previous result that $\hat{k}$ actually evaluates the first eigenvalue which is above a threshold related to the largest eigenvalue of the noise $\hat{\rho} - \rho$.

V. NUMERICAL PERFORMANCE OF THE PROCEDURE

In this section we implement an efficient procedure to solve the optimization problem (9) from the previous section. Indeed, the estimator $\hat{\rho}$ will be considered as an input from now on. It is computed very efficiently via linear operations and the real issue here is how to project this estimator on a subspace of matrices with smaller unknown rank in an optimal way. We are interested in two aspects of the method: its ability to select the rank correctly and the correct choice of the penalty. First, we explore the penalized procedure on example data and tune the parameter ν conveniently. In this way, we evaluate the performance of the linear estimator and of the rank selector. We then apply the method on real data sets.

The algorithm for solving (9) is given in [25]. We adapt it to our context and obtain the simple procedure.

Algorithm:

Inputs: The linear estimator $\hat{\rho}$ and a positive value of the tuning parameter ν

Outputs: An estimation $\hat{k}$ of the rank and an approximation $\hat{R}_{\hat{k}}$ of the state matrix.

Step 1. Compute the eigenvectors $V = [v_1, \dots, v_{2^n}]$ corresponding to the eigenvalues of the matrix $\hat{\rho}^\star\hat{\rho}$ sorted in decreasing order.

Step 2. Let $U = \hat{\rho}V$.

Step 3. For $k = 1, \dots, 2^n$, let V_k and U_k be the restrictions to their k first columns of V and U, respectively.

Step 4. For $k = 1, \dots, 2^n$, compute the estimators $\hat{R}_k = U_k V_k^\star$.

Step 5. Compute the final solution $\hat{R}_{\hat{k}}$, where, for a given positive value ν, $\hat{k}$ is defined as the minimizer in k over $\{1, \dots, 2^n\}$ of

$$\left\|\hat{R}_k - \hat{\rho}\right\|_F^2 + \nu \cdot k.$$

The constant k in the above procedure plays the role of the rank and then $\hat{R}_k$ is the best approximation of $\hat{\rho}$ with a matrix of rank k. As a consequence, this approach provides an estimation of both of the matrix ρ and of its rank d by $\hat{R}_{\hat{k}}$ and $\hat{k}$, respectively.

Obviously, this solution is strongly related to the value of the tuning parameter ν. Before dealing with how to calibrate this parameter, let us present a property that should help us to reduce the computational cost of the method.

The above algorithm is simple but requires the computation of 2^n matrices in Step 3 and Step 4. We present here an alternative which makes possible to compute only the matrix $\hat{R}_k$ that corresponds to $k = \hat{k}$, and then reduce the storage requirements.

Remember that $\hat{k}$ is the value of k minimizing the quantity in Step 5 of the above algorithm. Let $\lambda_1(\hat{\rho}) > \lambda_2(\hat{\rho}) > ...$ be the ordered eigenvalues of $\sqrt{\hat{\rho}^\star\hat{\rho}}$. According to [9, Proposition 1], it turns out that $\hat{k}$ is the largest k such that the eigenvalue $\lambda_k(\hat{\rho})$ exceeds the threshold $\sqrt{\nu}$:

$$\hat{k} = \max\{k : \lambda_k(\hat{\rho}) \geq \sqrt{\nu}\}. \tag{10}$$

As a consequence, one can compute the eigenvalues of the matrix $\sqrt{\hat{\rho}^\star\hat{\rho}}$ and set $\hat{k}$ as in (10). This value is then used to compute the best solution $\hat{R}_{\hat{k}}$ thanks to Step 1 to Step 4 in the above algorithm, with the major difference that we restrict Step 3 and Step 4 to only $k = \hat{k}$.

Example Data

We build artificial density matrices ρ with a given rank d in $\{1, \dots, 6\}$. These matrices are $2^n \times 2^n$ with $n = 4$ and 5. To construct such a matrix, we take ρ as $D_d = \frac{1}{d}diag(1...10...0)$, the diagonal matrix with its first d diagonal terms equal $1/d$, whereas the others equal zero.

We aim at testing how often we select the right rank based on the method illustrated in (10) as a function of the rank d, and of the number m of repetitions of the measurements we have in hand. Our algorithm depends on the tuning parameter ν. We use and compare two different values of the threshold ν: denote by $\nu_n^{(1)}$ and $\nu_n^{(2)}$ the values the parameter ν provided in Theorem 4 and Corollary 5 respectively. That is,

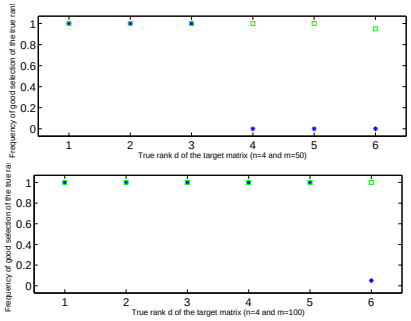
$$\nu_n^{(1)} = \|\hat{\rho} - \rho\|^2 \quad \text{and} \quad \nu_n^{(2)} = 32(1+\theta)\left(\frac{4}{3}\right)^n \frac{n\log(2)}{m}. \tag{11}$$

As established in Theorem 4, if the tuning parameter ν is of order of the parameter $\nu_n^{(1)}$, the solution of our algorithm is an accurate estimate of ρ. We emphasize the fact that $\nu_n^{(1)}$ is nothing but the estimation error of our linear estimator $\hat{\rho}$. We study this error below. On the other hand, the parameter $\nu_n^{(2)}$ is an upper bound of $\nu_n^{(1)}$ that ensures that the accuracy of estimation remains valid with high probability (*cf.* Corollary 5). The main advantage of $\nu_n^{(2)}$ is that it is completely known by the practitioner, which is not the case of $\nu_n^{(1)}$.

Rank estimation. Our first goal consists in illustrating the estimation power of our method in selecting the true rank d based on the calibrations of ν given by (11). We provide some conclusions on the number of repetitions m of the measurements needed to recover the right rank as a function of this rank. Figure 1 illustrates the evolution of the selection power of our method based on $\nu_n^{(1)}$ (blue stars) on the one hand, and based on $\nu_n^{(2)}$ (green squares) on the other hand.

Two conclusions can be made. First, the method based on $\nu_n^{(1)}$ is powerful. It almost always selects the right rank. It outperforms the algorithm based on $\nu_n^{(2)}$. This is an interesting observation. Indeed, $\nu_n^{(2)}$ is an upper bound of $\nu_n^{(1)}$. It seems that this bound is too large and can be used only for particular settings. Note however

FIG. 1: (Color online). Frequency of good selection of the true rank d, based on (10) with $\nu = \nu_n^{(1)}$ (green squares) and with $\nu = \nu_n^{(2)}$ (blue stars). The results are established on 20 repetitions. A value equal to 1 in the y-axis means that the method always selects the good rank, whereas 0 means that it always fails. First: $m = 50$ measurements – Second: $m = 100$ measurements



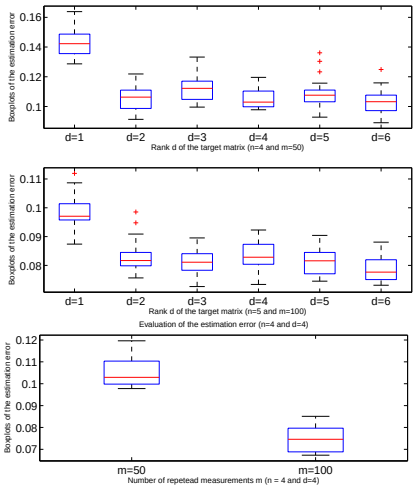
that in the variable selection literature, the calibration of the tuning parameter is a major issue and is often fixed by Cross-Validation (or other well-known methods). We have chosen here to illustrate only the result based on our theory and we will provide later an instruction to properly calibrate the tuning parameter ν.

The second conclusion goes in the direction of this instruction. As expected, the selection power of the method (based on both $\nu_n^{(1)}$ and $\nu_n^{(2)}$) increases when the number of repetition m of the measurements increases. Compare the figure for $m = 50$ repetitions to the figure for $m = 100$ repetitions in Figure 1. Moreover, for ranks smaller than some values, the methods always select the good rank. For larger ranks, they perform poorly. For instance with $m = 50$ (a small number of measurements), we observe that the algorithm based on $\nu_n^{(2)}$ performs poorly when the rank $d \geq 4$, whereas the algorithm based on $\nu_n^{(1)}$ is still excellent.

Actually, the bad selection when d is large does not mean that the methods perform poorly. Indeed our definition of the matrix ρ implies that the eigenvalues of the matrix decrease with d. They equal to $1/d$. Therefore, if $\sqrt{\nu}$ is of the same order as $1/d$, finding the exact rank becomes difficult since this calibration suggests that the eigenvalues are of the same order of magnitude as the error. Hence, in such situation, our method adapts to the context and find the effective rank of ρ. As an example, let consider our study with $n = 4$, $m = 50$ and $d = 6$. Based on 20 repetitions of the experiment, we obtain a maximal value of $\nu_n^{(1)} = \|\hat{\rho} - \rho\|^2$ equal to 0.132. This value is quite close to 0.167, the value of the eigenvalues of ρ. This explains the fact that our method based on $\nu_n^{(1)}$ failed in one iteration (among 20) to find the good rank. In this context $\nu_n^{(2)}$ is much larger than 0.167 and then our method does not select the correct rank with this calibration in this setting.

Let us also mention that we explored numerous experiments with other choices of the density matrix ρ. The same conclusion remains valid. When the error of the linear estimator $\hat{\rho}$ which is given by $\nu_n^{(1)} = \|\hat{\rho} - \rho\|^2$ is close to the square of the smallest eigenvalue of ρ, finding the exact rank is a difficult task. However, the method based on $\nu_n^{(1)}$ is still good, but fails sometimes. We produced data from physically meaningful states: the GHZ-state and the W-state for $n = 4$ qubits, as well as a statistical mixture $M_{d,p} = p * GHZ + (1 - p) * D_d$, for $d = 3$ and $p = 0.2$ Note that the rank of $M_{d,p}$ is 4.

FIG. 2: (Color online). Evaluation of the operator norm $\sqrt{\nu_n^{(1)}} = \|\hat{\rho} - \rho\|$. The results are established on 20 repetitions. Above: $n = 4$, $m = 50$ repetitions of the measurements ; we compare the errors when d takes values betwenn 1 and 6 – Middle: $n = 5$, $m = 100$; we compare the errors when d takes values between 1 and 6 – Below: the rank equals $d = 4$ and compare the error for $m = 50$ and 100.



Calibration of the tuning parameter ν. The quantity $\nu_n^{(1)} = \|\hat{\rho} - \rho\|^2$ seems to be very important to provide a good estimation of the rank d (or more precisely of the effective rank). Then it is interesting to observe how this quantity behaves. Figure 2 (Above $m = 50$ and $d = 4$, and Middle $m = 100$ and $d = 5$) illustrates how $\nu_n^{(1)}$ varies when the rank increases. Except for $d = 1$, it seems that the value of $\nu_n^{(1)}$ is quite stable. These graphics are obtained with particular values of the parameters m and d, but similar illustrations can be obtained if these parameters change.

The main observation according to the parameter ν is

that it decreases with m (see Figure 2 - Below) and is actually independent of the rank d (with some strange behavior when $d = 1$). This is in accordance with the definition of $\nu_n^{(2)}$ which is an upper bound of $\nu_n^{(1)}$.

Real-data analysis

In the next paragraph, we propose a 2-steps instruction for practitioners to use our method in order to estimate a matrix ρ (and its rank d) obtained from the data $R^{\mathbf{a},i}$ we have in hand with $\mathbf{a} \in \{x, y, z\}$ and $i \in \{1, \ldots, m\}$.

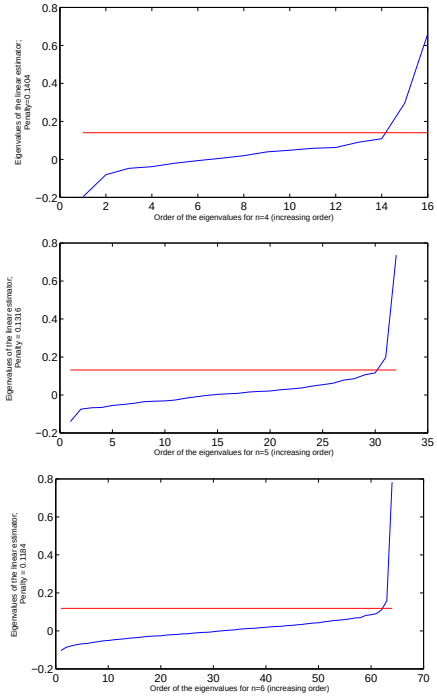
Real Data Algorithm:
Inputs: for any measurement $\mathbf{a} \in \{x, y, z\}$ we observe $R^{\mathbf{a},i}$, $i = 1, \ldots, m$.
Outputs: $\hat{k}$ and $\hat{R}_{\hat{k}}$, estimations of the rank d and ρ respectively.
The procedure starts with the linear estimator $\hat{\rho}$ and consists in two steps:

Step A. Use $\hat{\rho}$ to simulate repeatedly data with the same parameters n and m as the original problem. Use the data to compute synthetic linear estimators and the mean operator norm of these estimators. They provide an evaluation of the tuning parameter $\tilde{\nu}_n^{(1)}$.

Step B. Find $\hat{k}$ using (10) and construct $\hat{R}_{\hat{k}}$.

We have applied the method to real data sets concerning systems of 4 to 6 ions, which are Smolin states further manipulated. In Figure 3 we plot the eigenvalues of the linear estimator and the threshold given by the penalty. In each case, the method selects a rank equal to 2.

FIG. 3: (Color online). Eigenvalues of the linear estimator in increasing order and the penalty choice; $m = 100$ and $n = 4$, 5 or 6, respectively.



VI. CONCLUSIONS

We present here a method for reconstructing the quantum state of a system of n qubits from all measurements, each repeated m times. Such an experiment produce a huge amount of data to exploit in efficient way.

We revisit the inversion method and write an explicit formula for what is here called the linear estimator. This procedure does not produce a proper quantum state and has other well-known inconvenients. We consider projection of this state on the subspace of matrices with fixed rank and give an algorithm to select from data the rank which best suits the given quantum system. The method is very fast, as it comes down to choosing the eigenvalues larger than some threshold, which also appears in the penalty term. This threshold is of the same order as the error of the linear estimator. Its computation is crucial for good selection of the correct rank and it can be time consuming. Our algorithm also provides a consistent estimator of the true rank of the quantum system.

Our theoretical results provide a penalty term ν which has good asymptotic properties but our numerical results show that it is too large for most examples. Therefore we give an idea about how to evaluate closer the threshold by Monte-Carlo computation. This step can be time con-

suming but we can still improve on numerical efficiency (parallel computing, etc.).

In practice, the method works very well for large systems of small ranks, with significant eigenvalues. Indeed, there is a trade-off between the amount of data which will give small estimation error (and threshold) and the smallest eigenvalue that can be detected above this threshold. Neglecting eigenvalues comes down to reducing the number of parameters to estimate and reducing the variance, whereas large rank will increase the number of parameters and reduce the estimation bias.

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VII. APPENDIX

Proof of Proposition 2 Actually, we can compute

$$(\mathbf{P}^T\mathbf{P})_{\mathbf{b}_1,\mathbf{b}_2} = \sum_{(\mathbf{r},\mathbf{a})} \prod_{j\notin E_{\mathbf{b}_1}} r_j\,\mathbf{I}(a_j=b_{1,j}) \prod_{k\notin E_{\mathbf{b}_2}} r_k\,\mathbf{I}(a_k=b_{2,k}).$$

In case $\mathbf{b}_1=\mathbf{b}_2=\mathbf{b}$, we have

$$\begin{aligned}(\mathbf{P}^T\mathbf{P})_{\mathbf{b},\mathbf{b}} &= \sum_{(\mathbf{r},\mathbf{a})} \left(\prod_{j\notin E_{\mathbf{b}}} r_j\,\mathbf{I}(a_j=b_j)\right)^2 \\ &= \sum_{(\mathbf{r},\mathbf{a})} \prod_{j\notin E_{\mathbf{b}}} \mathbf{I}(a_j=b_j) = 3^{d(\mathbf{b})}2^n.\end{aligned}$$

In case $\mathbf{b}_1\neq\mathbf{b}_2$, we have either $E_{\mathbf{b}_1}=E_{\mathbf{b}_2}$ or $E_{\mathbf{b}_1}\neq E_{\mathbf{b}_2}$. If we suppose $E_{\mathbf{b}_1}=E_{\mathbf{b}_2}$,

$$\prod_{j\notin E_{\mathbf{b}_1}} r_j\,\mathbf{I}(a_j=b_{1,j}) \prod_{k\notin E_{\mathbf{b}_2}} r_k\,\mathbf{I}(a_k=b_{2,k}) = 0.$$

Indeed, if this is not 0 it means $\mathbf{a}=\mathbf{b}_1=\mathbf{b}_2$ outside the set E_{b_1}, that is $\mathbf{b}_1=\mathbf{b}_2$ which contradicts our assumption.

If we suppose $E_{\mathbf{b}_1}\neq E_{\mathbf{b}_2}$, we have either $\mathbf{b}_1\neq\mathbf{b}_2$ on the set $E^C_{\mathbf{b}_1}\cap E^C_{\mathbf{b}_1}$ and in this case one indicator in the product is bound to be 0, or we have $\mathbf{b}_1\neq\mathbf{b}_2$ on the set $E^C_{\mathbf{b}_1}\cap E^C_{\mathbf{b}_1}$. In this last case, take j_0 in the symmetric difference of sets $E_{\mathbf{b}_1}\Delta E_{\mathbf{b}_2}$. Then,

$$\begin{aligned}&(\mathbf{P}^T\mathbf{P})_{\mathbf{b}_1,\mathbf{b}_2} \\ &= \sum_{(\mathbf{r},\mathbf{a})} \prod_{j\notin E_{\mathbf{b}_1}} r_j\,\mathbf{I}(a_j=b_{1,j}) \prod_{k\notin E_{\mathbf{b}_2}} r_k\,\mathbf{I}(a_k=b_{2,k}) \\ &= \sum_{(\mathbf{r},\mathbf{a})} \prod_{j\notin E_{\mathbf{b}_1}} \mathbf{I}(a_j=b_{1,j}) \prod_{k\notin E_{\mathbf{b}_2}} \mathbf{I}(a_k=b_{2,k}) \prod_{j\in E_{\mathbf{b}_1}\Delta E_{\mathbf{b}_2}} r_j \\ &= \sum_{r_{j_0}\in\{-1,1\}} r_{j_0} \sum_{\mathbf{r}\neq r_{j_0}} \sum_{\mathbf{a}} \prod_{j\notin E_{\mathbf{b}_1}} \mathbf{I}(a_j=b_{1,j}) \\ &\quad \prod_{k\notin E_{\mathbf{b}_2}} \mathbf{I}(a_k=b_{2,k}) \prod_{j\in E_{\mathbf{b}_1}\Delta E_{\mathbf{b}_2}/j_0} r_j = 0.\end{aligned}$$

□

Proof of Proposition 3 It is easy to see that $\hat{\vec{\rho}}$ is an unbiased estimator. We write its variance as follows:

$$\begin{aligned}&Var(\hat{\rho}_{\mathbf{b}}) \\ &= \frac{1}{3^{2d(\mathbf{b})}4^n} \sum_{\mathbf{a}\in\mathcal{E}^n} Var\left(\sum_{\mathbf{r}\in\mathcal{R}^n} \frac{1}{m}\sum_{i=1}^m \delta_{R^{\mathbf{a},i},\mathbf{r}}\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}\right) \\ &= \frac{1}{3^{2d(\mathbf{b})}4^n m^2} \sum_{\mathbf{a}\in\mathcal{E}^n}\sum_{\mathbf{r}\in\mathcal{R}^n} m p_{(\mathbf{r},\mathbf{a})}\mathbf{P}^2_{(\mathbf{r},\mathbf{a}),\mathbf{b}} \\ &\quad -\frac{1}{3^{2d(\mathbf{b})}4^n m^2} \sum_{\mathbf{a}\in\mathcal{E}^n} m\left(\sum_{\mathbf{r}\in\mathcal{R}^n} p_{(\mathbf{r},\mathbf{a})}\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}\right)^2 \\ &= \frac{1}{3^{2d(\mathbf{b})}4^n m} \sum_{(\mathbf{r},\mathbf{a})\in(\mathcal{R}^n\times\mathcal{E}^n)} p_{(\mathbf{r},\mathbf{a})} \prod_{j\notin E_{\mathbf{b}}} \mathbf{I}(a_j=b_j) \\ &\quad -\frac{1}{m}\sum_{\mathbf{a}\in\mathcal{E}^n}\left(\frac{1}{3^{d(\mathbf{b})}2^n}\sum_{\mathbf{r}\in\mathcal{R}^n} p_{(\mathbf{r},\mathbf{a})} \prod_{j\notin E_{\mathbf{b}}} r_j\mathbf{I}(a_j=b_j)\right)^2 \\ &\leq \frac{1}{3^{d(\mathbf{b})}4^n m}.\end{aligned}$$

Finally, let us prove the last point. We will use the following result due to [27].

Theorem 7 (Matrix Hoeffding's inequality [27]) *Let X_1, ..., X_p be independent centered self-adjoint random matrices with values in $\mathbb{C}^{d\times d}$, and let us assume that there are deterministic self-adjoint matrices A_1, ..., A_p such that, for all $i_in\{1,...,p\}$, $A_i^2 - X_i^2$ is a.s. nonnegative. Then, for all $t>0$,*

$$\mathbb{P}\left(\left\|\sum_{i=1}^p X_i\right\|^2 \geq t\right) \leq d\exp\left(\frac{-t^2}{8\sigma^2}\right)$$

where $\sigma^2 = \|\sum_{k=1}^p A_k^2\|$.

We have:

$$\begin{aligned}\hat{\rho}-\rho &= \sum_{\mathbf{b}}(\hat{\rho}_{\mathbf{b}}-\rho_{\mathbf{b}})\sigma_{\mathbf{b}}\\ &= \sum_{\mathbf{b}}\sum_{\mathbf{r}}\sum_{\mathbf{a}}\frac{\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}}{3^{d(\mathbf{b})}2^n}(\hat{p}_{\mathbf{r},\mathbf{a}}-p_{\mathbf{r},\mathbf{a}})\sigma_{\mathbf{b}}\\ &= \sum_{\mathbf{b}}\sum_{\mathbf{r}}\sum_{\mathbf{a}}\sum_{i}\frac{\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}}{3^{d(\mathbf{b})}2^n m}(\mathbb{1}_{R^{i,\mathbf{a}}=\mathbf{r}}-p_{\mathbf{r},\mathbf{a}})\sigma_{\mathbf{b}}\\ &= \sum_{\mathbf{a}}\sum_{i}\underbrace{\sum_{\mathbf{b}}\sum_{\mathbf{r}}\frac{\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}}{3^{d(\mathbf{b})}2^n}(\mathbb{1}_{R^{i,\mathbf{a}}=\mathbf{r}}-p_{\mathbf{r},\mathbf{a}})\sigma_{\mathbf{b}}}_{=:X_{i,\mathbf{a}}}.\end{aligned}$$

Note that the $X_{i,\mathbf{a}}$, for $i\in\{1,...,m\}$ and $\mathbf{a}\in\mathcal{E}^n$, are iid self-adjoint centered random matrices. Moreover, we have:

$$\begin{aligned}\|X_{i,\mathbf{a}}\| &= \left\|\sum_{\mathbf{b}}\sum_{\mathbf{r}}\frac{\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}}{3^{d(\mathbf{b})}2^n m}(\mathbb{1}_{R^{i,\mathbf{a}}=\mathbf{r}}-p_{\mathbf{r},\mathbf{a}})\sigma_{\mathbf{b}}\right\|\\ &\le \sum_{\mathbf{b}}\sum_{\mathbf{r}}\left|\frac{\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}}{3^{d(\mathbf{b})}2^n m}\right||\mathbb{1}_{R^{i,\mathbf{a}}=\mathbf{r}}-p_{\mathbf{r},\mathbf{a}}|\underbrace{\|\sigma_{\mathbf{b}}\|}_{=1}\\ &= \sum_{\mathbf{b}}\left|\frac{\mathbf{P}_{(\mathbf{r},\mathbf{a}),\mathbf{b}}}{3^{d(\mathbf{b})}2^n m}\right|\underbrace{\sum_{\mathbf{r}}|\mathbb{1}_{R^{i,\mathbf{a}}=\mathbf{r}}-p_{\mathbf{r},\mathbf{a}}|}_{\le 2}\\ &= \frac{2}{2^n m}\sum_{\mathbf{b}}\frac{1}{3^{d(\mathbf{b})}}\prod_{j\notin E_{\mathbf{b}}}\mathbb{1}_{a_j=b_j}\\ &\le \frac{2}{2^n m}\sum_{\ell=0}^{n}\sum_{\substack{\mathbf{b}\text{ such that}\\ d(\mathbf{b})=\ell\\ \forall j\notin E_{\mathbf{b}},\,a_j=b_j}}\frac{1}{3^\ell}\\ &= \frac{2}{2^n m}\sum_{\ell=0}^{n}\binom{\ell}{n}\frac{1}{3^\ell} = \frac{2}{2^n m}\left(1+\frac{1}{3}\right)^n = \frac{2}{m}\left(\frac{2}{3}\right)^n.\end{aligned}$$

This proves that $A_{i,\mathbf{a}}^2-X_{i,\mathbf{a}}^2$ is nonnegative where $A_{i,\mathbf{a}}=\frac{2}{m}\left(\frac{2}{3}\right)^n I$. So we can apply Theorem 7, we have:

$$\sigma^2 = \|\sum_{i,\mathbf{a}}A_{i,\mathbf{a}}^2\| = \frac{4}{m}\left(\frac{4}{3}\right)^n$$

and so

$$\begin{aligned}&\mathbb{P}\left(\|\hat{\rho}-\rho\|^2\ge t\right) = \mathbb{P}\left(\left\|\sum_{i,\mathbf{a}}X_{i,\mathbf{a}}\right\|^2\ge t\right)\\ &\le\ 2^n\exp\left(\frac{-t^2 m}{32}\left(\frac{3}{4}\right)^n\right).\end{aligned}$$

We put

$$\varepsilon = 2^n\exp\left(\frac{-t^2 m}{32}\left(\frac{3}{4}\right)^n\right),$$

this leads to:

$$\mathbb{P}\left(\|\hat{\rho}-\rho\|^2\ge 4\sqrt{2\left(\frac{4}{3}\right)^n\frac{n\log(2)-\log(\varepsilon)}{m}}\right)\le\varepsilon.$$

□

Proof of Theorem 4 From the definition (8) of our estimator, we have, for any Hermitian, positive semi-definite matrix R,

$$\|\hat{\rho}_\nu-\hat{\rho}\|_F^2+\nu\text{rank}(\hat{\rho}_\nu)\ \le\ \|R-\hat{\rho}\|_F^2+\nu\text{rank}(R).$$

We deduce that

$$\begin{aligned}&\|\hat{\rho}_\nu-\rho\|_F^2\\ \le\ &\|R-\rho\|_F^2+2\text{Tr}((\hat{\rho}-\rho)^\star(R-\hat{\rho}_\nu))\\ &+\nu(\text{rank}(R)-\text{rank}(\hat{\rho}_\nu))\\ \le\ &\|R-\rho\|_F^2+2\nu\text{rank}(R)+2\|\hat{\rho}-\rho\|\times\|R-\hat{\rho}_\nu\|_1\\ &-\nu(\text{rank}(R)+\text{rank}(\hat{\rho}_\nu)).\end{aligned}$$

Further on, we have

$$\begin{aligned}&\|R-\hat{\rho}_\nu\|_1\\ \le\ &(\text{rank}(R)+\text{rank}(\hat{\rho}_\nu))^{1/2}\|R-\hat{\rho}_\nu\|_F\\ \le\ &(\text{rank}(R)+\text{rank}(\hat{\rho}_\nu))^{1/2}(\|\rho-\hat{\rho}_\nu\|_F+\|R-\rho\|_F)\end{aligned}$$

We apply two times the inequality $2A\cdot B\le\epsilon A^2+\epsilon^{-1}B^2$ for any real numbers A, B and $\epsilon>0$. We actually use $\epsilon=1+\theta/2$ and $\epsilon=\theta/2$, respectively, and get

$$\begin{aligned}&\|\hat{\rho}_\nu-\rho\|_F^2\\ \le\ &\|R-\rho\|_F^2+2\nu\text{rank}(R)-\nu(\text{rank}(R)+\text{rank}(\hat{\rho}_\nu))\\ &+(1+\theta)(\text{rank}(R)+\text{rank}(\hat{\rho}_\nu))\|\hat{\rho}-\rho\|^2\\ &+(1+\frac{\theta}{2})^{-1}\|\hat{\rho}_\nu-\rho\|_F^2+(\frac{\theta}{2})^{-1}\|R-\rho\|_F^2.\end{aligned}$$

By rearranging the previous terms, we get that for any Hermitian matrix R

$$\|\hat{\rho}_\nu-\rho\|_F^2\le c^2(\theta)\|R-\rho\|_F^2+2c(\theta)\nu\text{rank}(R),$$

provided that $\nu\ge(1+\theta)\|\hat{\rho}-\rho\|^2$. By following [9], the least possible value for $\|R-\rho\|_F^2$ is $\sum_{j>k}\lambda_j^2(\rho)$ if the matrices R have rank k. Moreover, this value is obviously attained by the projection of ρ on the space of the eigenvectors associated to the k largest eigenvalues. This helps us conclude the proof of the theorem. □

Proof of Corollary 6 Recall that $\hat{k}$ is the largest k such that $\lambda_k(\hat{\rho})\ge\sqrt{\nu}$. We have

$$\mathbb{P}(\hat{k}\ne k)=\mathbb{P}(\lambda_k(\hat{\rho})\le\sqrt{\nu}\text{ or }\lambda_{k+1}(\hat{\rho})\ge\sqrt{\nu}).$$

Now, $\lambda_k(\rho) \leq \lambda_k(\hat{\rho}) + \|\hat{\rho} - \rho\|$ and $\lambda_{k+1}(\rho) \geq \lambda_{k+1}(\hat{\rho}) - \|\hat{\rho} - \rho\|$. Thus,

$$\mathbb{P}(\hat{k} \neq k) \leq \mathbb{P}(\|\hat{\rho} - \rho\| \geq \min\{\lambda_k(\rho) - \sqrt{\nu}, \sqrt{\nu} - \lambda_{k+1}(\rho)\})$$

and this is smaller than $\mathbb{P}(\|\hat{\rho} - \rho\| \geq \delta\sqrt{\nu})$, by the assumptions of the Corollary. □

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