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# RANK PENALIZED ESTIMATION OF A QUANTUM SYSTEM

PIERRE ALQUIER<sup>1,4</sup>, CRISTINA BUTUCEA<sup>2,4</sup>, MOHAMED HEBIRI<sup>2</sup>, KATIA MEZIANI<sup>2,3</sup>

ABSTRACT. We introduce a new method to reconstruct the quantum matrix  $\bar{\rho}$  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  $\rho$  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 state 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  $dn(3/4)^n/m$  and consistency for the estimator of the rank. The proposed methodology is computationally efficient and is illustrated with synthetic and real data sets.

## CONTENTS

1. Introduction	1
2. Basic notation and setup	3
3. Identifiability of the model	4
4. Estimation procedure and error bounds	6
4.1. Linear estimator	6
4.2. Rank penalized estimator	7
5. Numerical performance of the procedure	8
6. Appendix	13
References	15

## 1. INTRODUCTION

The experimental study of quantum mechanical systems has made huge progress recently. Producing and manipulating large quantum mechanical systems is easier to achieve. Following such an experimental setup, we suppose that we have a source of quantum systems which are identically prepared in some state. The goal is to reconstruct this state via Quantum State Tomography (QST). The QST is an experimental process where each system is repeatedly measured with different elements of a projector-valued measure (PVM).

Most popular methods for estimating the state from such data are: linear inversion [20], maximum likelihood [3], [11], [6] and Bayesian inference [1], [2], [5] (see also 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 [13]

the penalty is the Von Neumann entropy of the state, while [9], [10] use the  $\mathbb{L}_1$  penalty to implement 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. Indeed, more experiments deal nowadays with entanglement and the low-rank assumption does not correspond to such experiments. Instead, all measurements are implemented and for each one  $m$  independent, identically distributed (i.i.d.) random variables are available. 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 state matrix of a  $n$ -qubits system, our final procedure has the risk (squared Frobenius norm) bounded by  $dn(3/4)^n/m$ , 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 project the output on the set of density matrices, with the result that the distance to the true state can only be decreased in the proper norm.

Moreover, the rank of the large density matrix is an indicator of entanglement in the system. We shall indicate how to project the linear estimator of the state on the space of matrices 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 state 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 [4], [16].

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 state 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 synthetic data and apply them to real-data, in Section 5. The last section is dedicated to proofs.

## 2. BASIC NOTATION AND SETUP

We have a system of  $n$  qubits. This system is represented by a  $2^n \times 2^n$  matrix  $\bar{\rho}$ , with coefficients in  $\mathbb{C}$ . This matrix is Hermitian  $\bar{\rho}^* = \bar{\rho}$ , semidefinite positive  $\bar{\rho} \geq 0$  and has  $\text{Tr}(\bar{\rho}) = 1$ . It is the “state matrix” which fully describes the system of  $n$  particles. The objective is to estimate  $\bar{\rho}$ , from measurements of many independent systems, identically prepared in this state.

For each system, the experiment provides random data from separate measurements  $\sigma_x, \sigma_y, \sigma_z$  on each mode, where we use here the classical notation for the Pauli matrices. The collection of measurements which are performed writes

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

where  $\mathbf{a} = (a_1, \dots, a_n)$  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:

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

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

For the sake of simplicity, we propose to introduce the notation

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

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

The tomographic inversion method for reconstructing  $\bar{\rho}$  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

$$(3) \quad \hat{p}(\mathbf{a}, \mathbf{r}) = \text{Tr}(\hat{\rho} \cdot P_{\mathbf{r}}^{\mathbf{a}}).$$

It is known in statistics as the method of moments.

We shall use in the sequel the following notation:  $\|A\|_F^2 = \text{Tr}(A^*A)$  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  $\bar{\rho}$ . 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

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

where the minimum is taken over all Hermitian, positive semidefinite matrices  $R$ . This 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 [7, 12, 17, 19] and Chapter 9 in [15]. Here, we follow the computation in [7].

In order to give such explicit inversion formula we first change the coordinates of the matrix  $\bar{\rho}$  into a vector  $\rho \in \mathbb{R}^{4^n}$  on a convenient basis. The linear inversion also gives information about the quality of each estimator of the coordinates in  $\rho$ . Thus we shall see that we have to perform all measurements  $\sigma_{\mathbf{a}}$  in order to recover (some) information on each coordinate of  $\rho$ . 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 Guta, Monz (private communication) addresses the same issue via the maximum likelihood procedure. Other adaptive methods include matrix completion for low-rank matrices [8, 9, 10, 14] and for matrices with small Von Neumann entropy [13].

### 3. 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 change coordinates and express matrix  $\bar{\rho}$  on the basis provided by the measurements. More precisely, 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)

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

Then, we have the following decomposition:

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

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

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

Finally, elementary computations lead to  $\text{Tr}(IP_s^t) = 1$  for any  $s \in \{-1, 1\}$  and  $t \in \{x, y, z\}$ , while  $\text{Tr}(\sigma_t P_s^{t'}) = s \mathbf{1}_{t=t'}$  for any  $s \in \{-1, 1\}$  and  $(t, t') \in \{x, y, z\}^2$ .

For any  $\mathbf{b} \in \mathcal{M}^n$ , we denote by  $E_{\mathbf{b}} = \{j \in \{1, \dots, n\} : b_j = I\}$ . The above calculation have proved the following result.

**Proposition 3.1.** *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,  $\mathbf{b} = (x, \dots, x)$ , then the associated set  $E_{\mathbf{b}}$  is empty and  $\mathbb{P}(R^{(x, \dots, x)} = \mathbf{r})$  is the only probability depending on  $\rho_{(x, \dots, x)}$  among other coefficients. Therefore, only the measurement  $(\sigma_x, \dots, \sigma_x)$  will bring information on this coefficient. Whereas, if  $\mathbf{b} = (I, I, x, \dots, x)$ , the set  $E_{\mathbf{b}}$  contains 2 points. There are  $3^2$  measurements  $((\sigma_x, \dots, \sigma_x), \dots, (\sigma_z, \sigma_z, \sigma_x, \dots, \sigma_x))$  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:

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

Our objective is to study the invertibility of the operator

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

Thanks to Proposition 3.1, 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:

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

and from Proposition 3.1 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  $\mathbf{P}\rho = \mathbf{p}$ . 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 3.2.** *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  $\mathbf{P}\rho = \mathbf{p}$  has a unique solution:*

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

In other words, we can reconstruct  $\rho = (\rho_{\mathbf{b}})_{\mathbf{b} \in \mathcal{M}^n}$  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.

#### 4. 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  $R^{\mathbf{a}, i}$ ,  $1 \leq i \leq m$ . 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  $p_{(\mathbf{r}, \mathbf{a})} = \mathbb{P}(R^{\mathbf{a}} = \mathbf{r})$ :

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

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

**4.1. Linear estimator.** We apply the inversion formula to the estimated vector  $\hat{\mathbf{p}}$ . Following Proposition 3.2 we can define:

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

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

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

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

**Proposition 4.1.** *The estimator  $\hat{\rho}$  of  $\rho$ , defined in (6) has the following properties:*

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

$$\text{Var}(\hat{\rho}_{\mathbf{b}}) \leq \frac{1}{3^{d(\mathbf{b})} 4^{nm}};$$

(3) for any  $\varepsilon > 0$ ,

$$\mathbb{P} \left( \max_{\mathbf{b} \in \mathcal{M}^n} |\hat{\rho}_{\mathbf{b}} - \rho_{\mathbf{b}}| \leq 2 \sqrt{2 \left( \frac{3}{4} \right)^n \frac{n \log(4) + \log \left( \frac{2}{\varepsilon} \right)}{m}} \right) \geq 1 - \varepsilon.$$

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  $|\hat{\rho} - \rho|_{\infty}$  which is valid with high probability. This quantity is related to  $\|\hat{\rho} - \bar{\rho}\|$  in a way that will be explained later on. The bound we obtain above depends on  $\log(4^n)$ , which is expected as  $4^n - 1$  is the total number of parameters of a full rank system. It also contains a more surprising factor  $(3/4)^n$  which is small when the system ( $n$ ) is large. This factor appears in the Hoeffding inequality that we use in order to prove this bound.

**4.2. Rank penalized estimator.** We investigate low-rank estimates of  $\bar{\rho}$  defined in (7). From now on, we follow closely the results in [7] which were obtained for a matrix regression model, with some differences as our model is different. Let us, for a positive real value  $\nu$  study the estimator:

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

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

$$(9) \quad \min_R \left[ \|R - \hat{\rho}\|_F^2 + \nu \cdot \text{rank}(R) \right] = \min_k \min_{R: \text{rank}(R)=k} \left[ \|R - \hat{\rho}\|_F^2 + \nu \cdot k \right].$$

An efficient algorithm is available to solve the minimization program (9) as a spectral-based decomposition algorithm provided in [18]. Let us denote by  $\hat{R}_k$  the matrix such that  $\|\hat{R}_k - \hat{\rho}\|_F^2 = \min_{R: \text{rank}(R)=k} \left[ \|R - \hat{\rho}\|_F^2 + \nu \cdot k \right]$ . 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 4.2.** For any  $\theta > 0$  put  $c(\theta) = 1 + 2/\theta$ . We have on the event  $\{\nu \geq (1 + \delta)\|\hat{\rho} - \bar{\rho}\|^2\}$  that

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

where  $\lambda_j(\bar{\rho})$  for  $j = 1, \dots, 2^n$  are the eigenvalues of  $\bar{\rho}$  ordered decreasingly.

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

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



Let us study the choice of  $\nu$  in Theorem 4.2 such that the probability of the event  $\{\nu \geq (1 + \theta)\|\hat{\rho} - \bar{\rho}\|^2\}$  is small. We have

$$\|\hat{\rho} - \bar{\rho}\| = \left\| \sum_{\mathbf{b} \in \mathcal{M}^n} (\hat{\rho}_{\mathbf{b}} - \rho_{\mathbf{b}}) \sigma_{\mathbf{b}} \right\| \leq \max_{\mathbf{b} \in \mathcal{M}^n} |\hat{\rho}_{\mathbf{b}} - \rho_{\mathbf{b}}|.$$

By putting together the previous theorem and Proposition 4.1, we get the following result:

**Corollary 4.3.** *For any  $\theta > 0$  put  $c(\theta) = 1 + 2/\theta$  and for some small  $\varepsilon > 0$  choose*

$$\nu(\theta, \varepsilon) = 8(1 + \theta) \left(\frac{3}{4}\right)^n \frac{n \log(4) + \log\left(\frac{2}{\varepsilon}\right)}{m}.$$

Then, we have

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

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  $\varepsilon > 0$ :

$$\|\hat{\rho}_{\nu} - \bar{\rho}\|_F^2 \leq 16c(\theta)d(1 + \theta) \left(\frac{3}{4}\right)^n \frac{n \log(4) + \log\left(\frac{2}{\varepsilon}\right)}{m},$$

with probability larger than  $1 - \varepsilon$ .

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

**Corollary 4.4.** *If there exists  $k$  such that  $\lambda_k(\bar{\rho}) > (1 + \delta)\sqrt{\nu}$  and  $\lambda_{k+1}(\bar{\rho}) < (1 - \delta)\sqrt{\nu}$  for some  $\delta$  in  $(0, 1]$ , then*

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

From an asymptotic point of view, this corollary means that, if  $d$  is the rank of the underlying matrix  $\bar{\rho}$ , then our procedure is consistent in finding the rank. Indeed, as  $\sqrt{\nu}$  is an upper bound of the norm  $\|\hat{\rho} - \bar{\rho}\|$ , 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  $\hat{\rho} - \bar{\rho}$ .

## 5. NUMERICAL PERFORMANCE OF THE PROCEDURE

In this section we implement an efficient procedure to solve the optimization problem (9) from the previous section. 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 synthetic data and tune the parameter  $\nu$  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 [18]. 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  $\nu$

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  $\hat{\rho}^* \hat{\rho}$  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  $\hat{R}_k = U_k V_k^*$ .

Step 5. Compute the final solution  $\hat{R}_{\hat{k}}$ , where, for a given positive value  $\nu$ ,  $\hat{k}$  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  $\hat{\rho}$  and of its rank  $d$  by  $\hat{R}_{\hat{k}}$  and  $\hat{k}$ , respectively.

Obviously, this solution is highly linked to value of the tuning parameter  $\nu$ . 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  $\lambda_1(\hat{\rho}) > \lambda_2(\hat{\rho}) > \dots$  be the ordered eigenvalues of  $\sqrt{\hat{\rho}^* \hat{\rho}}$ . According to [7, Proposition 1], it turns out that  $\hat{k}$  is the largest  $k$  such that the eigenvalue  $\lambda_k(\hat{\rho})$  exceeds the threshold  $\sqrt{\nu}$ :

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

As a consequence, one can compute the eigenvalues of the matrix  $\sqrt{\hat{\rho}^* \hat{\rho}}$  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  $k = \hat{k}$ .

### Synthetic Data

We build artificial state matrices  $\bar{\rho}$  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 define  $\bar{\rho}$  as 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  $\nu$ . We use and compare two different values of the threshold  $\nu$ : denote by  $\nu_n^{(1)}$

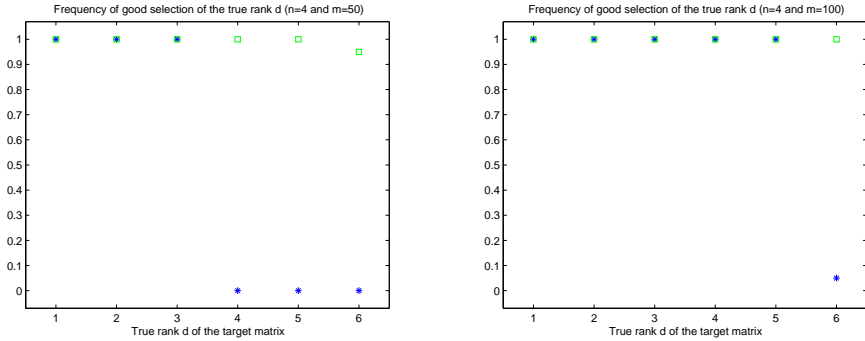
and  $\nu_n^{(2)}$  the values the parameter  $\nu$  provided in Theorem 4.2 and Corollary 4.3 respectively. That is,

$$(11) \quad \nu_n^{(1)} = \|\hat{\rho} - \bar{\rho}\|^2 \quad \text{and} \quad \nu_n^{(2)} = 8(1 + \theta) \left(\frac{3}{4}\right)^n \frac{n \log(4)}{m}.$$

As established in Theorem 4.2, if the tuning parameter  $\nu$  is of order of the parameter  $\nu_n^{(1)}$ , the solution of our algorithm is an accurate estimate of  $\bar{\rho}$ . 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 4.3). 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 the selecting the true rank  $d$  based on the calibrations of  $\nu$  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 5 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.

FIGURE 1. Frequency of good selection of the true rank  $d$  with respect to  $d$ , 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. Left:  $m = 50$  measurements – Right:  $m = 100$  measurements



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  $\nu_n^{(2)}$ -based algorithm. 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 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  $\nu$ .

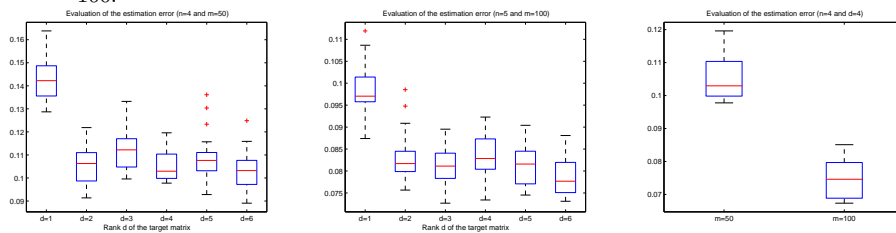
The second conclusion goes in the direction of this instruction. As expected, the selection power of the method (based on both  $\nu_n^{(1)}$  and  $\nu_n^{(2)}$ ) increases when the

number of repetition  $m$  of the measurements increases. Compare the left ( $m = 50$  repetitions) to the right ( $m = 100$  repetitions) picture in Figure 5. Moreover, up to a certain rank, 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  $\bar{\rho}$  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  $\bar{\rho}$ . 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  $\nu_n^{(1)} = \|\hat{\rho} - \bar{\rho}\|^2$  equal to 0.132. This value is quite close to 0.167, the value of the eigenvalues of  $\bar{\rho}$ . 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 the selection of the rank  $d$  is not efficient with this calibration and in this setting.

Let us also mention that we explored numerous experiments with other choices of the diagonal matrix  $\bar{\rho}$ . The same conclusion remains valid. When the error of the linear estimator  $\hat{\rho}$  which is given by  $\nu_n^{(1)} = \|\hat{\rho} - \bar{\rho}\|^2$  is close to the square of the smallest eigenvalue of  $\bar{\rho}$ , finding the exact rank is a difficult task. However, the method based on  $\nu_n^{(1)}$  is still good, but fails sometimes.

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



**Calibration of the tuning parameter  $\nu$ .** The quantity  $\nu_n^{(1)} = \|\hat{\rho} - \bar{\rho}\|^2$  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 5 (Left  $m = 50$  and  $d = 4$ , and Center  $m = 100$  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  $\nu$  is that it decreases with  $m$  (see Figure 5 - Right) 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  $\bar{\rho}$  (and its rank  $d$ ) obtained from the data  $R^{\mathbf{a},i}$  we have in hand with  $\mathbf{a} \in \{x, y, z\}$  and  $i \in \{1, \dots, m\}$ .

#### Real Data Algorithm:

Inputs: for any measurement  $\mathbf{a} \in \{x, y, z\}$  we observe  $R^{\mathbf{a},i}$ ,  $i = 1, \dots, m$ .

Outputs:  $\hat{k}$  and  $\hat{R}_{\hat{k}}$ , estimations of the rank  $d$  and  $\bar{\rho}$  respectively.

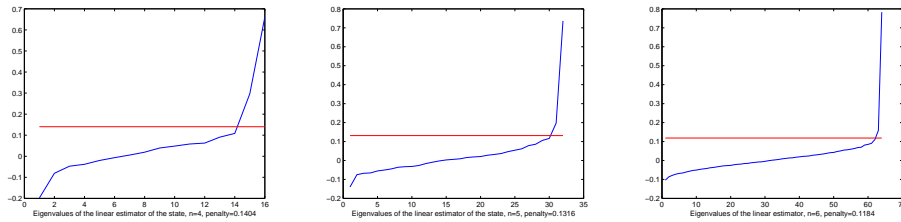
The procedure starts with the linear estimator  $\hat{\rho}$  and consists in two steps:

*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. In Figure 5 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, which possibly means that the system is not entangled.

FIGURE 3. Eigenvalues of the linear estimator in increasing order and the penalty choice;  $m = 100$  and  $n = 4, 5$  or  $6$ , respectively.



## 6. APPENDIX

*Proof of Proposition 3.2.* 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  $E_{\mathbf{b}_1}$ , 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  $E_{\mathbf{b}_1}^C \cap E_{\mathbf{b}_1}^C$  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  $E_{\mathbf{b}_1}^C \cap E_{\mathbf{b}_1}^C$ . 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 4.1.* It is easy to see that  $\hat{\rho}$  is an unbiased estimator. We write its variance as follows:

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

Now, let us fix  $\mathbf{b} \in \mathcal{M}^n$ . We have:

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

Note that the  $X^{i, \mathbf{a}}$  are all independent and satisfy  $\mathbb{E}(X^{i, \mathbf{a}}) = 0$  and

$$\begin{aligned}|X^{i, \mathbf{a}}| &\leq \sum_{\mathbf{r} \in \mathcal{R}^n} \underbrace{|\mathbf{P}_{(\mathbf{r}, \mathbf{a}), \mathbf{b}}|}_{\leq 1} \underbrace{|\mathbf{1}_{R^{\mathbf{a}, i} = \mathbf{r}} - p_{(\mathbf{r}, \mathbf{a})}|}_{\leq |\mathbf{1}_{R^{\mathbf{a}, i} = \mathbf{r}}| + |p_{(\mathbf{r}, \mathbf{a})}|} \\ &\leq 2.\end{aligned}$$

This means that we can use Hoeffding's inequality to get, for any  $\nu > 0$ ,

$$\begin{aligned}\mathbb{P}\left(\left|\sum_{i=1}^m \sum_{\mathbf{a} \in \mathcal{E}^n} X^{i, \mathbf{a}}\right| \geq \nu\right) &\leq 2 \exp\left(-\frac{\nu^2}{8m|\mathcal{E}^n|}\right) \\ \mathbb{P}\left(\left|\sum_{i=1}^m \sum_{\mathbf{a} \in \mathcal{E}^n} X^{i, \mathbf{a}}\right| \geq \nu\right) &\leq 2 \exp\left(-\frac{\nu^2}{8m3^n}\right) \\ \mathbb{P}\left(\left|\sum_{i=1}^m \sum_{\mathbf{a} \in \mathcal{E}^n} X^{i, \mathbf{a}}\right| \geq (3^{d(\mathbf{b})}2^n m)\nu\right) &\leq 2 \exp\left(-\frac{1}{8}3^{2d(\mathbf{b})}m\left(\frac{4}{3}\right)^n \nu^2\right) \\ \mathbb{P}(|\hat{\rho}_{\mathbf{b}} - \rho_{\mathbf{b}}| \geq \nu) &\leq 2 \exp\left(-\frac{1}{8}3^{2d(\mathbf{b})}m\left(\frac{4}{3}\right)^n \nu^2\right).\end{aligned}$$

A classical union bound argument leads to:

$$\begin{aligned}\mathbb{P}(\max_{\mathbf{b} \in \mathcal{M}^n} |\hat{\rho}_{\mathbf{b}} - \rho_{\mathbf{b}}| \geq \nu) &\leq \sum_{\mathbf{b} \in \mathcal{M}^n} \mathbb{P}(|\hat{\rho}_{\mathbf{b}} - \rho_{\mathbf{b}}| \geq \nu) \\ &\leq 2 \sum_{\mathbf{b} \in \mathcal{M}^n} \exp\left(-\frac{1}{8}3^{2d(\mathbf{b})}m\left(\frac{4}{3}\right)^n \nu^2\right) \\ &\leq 2 \cdot 4^n \exp\left(-\frac{1}{8}m\left(\frac{4}{3}\right)^n \nu^2\right).\end{aligned}$$

Putting, for a given  $\varepsilon > 0$ ,

$$2 \cdot 4^n \exp\left(-\frac{1}{8}m\left(\frac{4}{3}\right)^n \nu^2\right) = \varepsilon$$

leads to

$$\nu = 2\sqrt{2\left(\frac{3}{4}\right)^n \frac{n \log(4) + \log\left(\frac{2}{\varepsilon}\right)}{m}}.$$

□

*Proof of Theorem 4.2.* From the definition (8) of our estimator, we have, for any Hermitian, positive semi-definite matrix  $R$ ,

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

We deduce that

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

Further on, we have

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

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

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

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

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

provided that  $\nu \geq (1 + \theta)\|\hat{\rho} - \bar{\rho}\|^2$ . By following [7], the least possible value for  $\|R - \bar{\rho}\|_F^2$  is  $\sum_{j>k} \lambda_j^2(\bar{\rho})$  if the matrices  $R$  have rank  $k$ . Moreover, this value is obviously attained by the projection of  $\bar{\rho}$  on the space of the eigenvectors associated to the  $k$  largest eigenvalues. This helps us conclude the proof of the theorem.  $\square$

*Proof of Corollary 4.4.* Recall that  $\hat{k}$  is the largest  $k$  such that  $\lambda_k(\hat{\rho}) \geq \sqrt{\nu}$ . We have

$$\mathbb{P}(\hat{k} \neq k) = \mathbb{P}(\lambda_k(\hat{\rho}) \leq \sqrt{\nu} \text{ or } \lambda_{k+1}(\hat{\rho}) \geq \sqrt{\nu}).$$

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

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

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

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