

Uncertainty Quantification for Matrix Compressed Sensing and Quantum Tomography Problems

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Abstract: We construct minimax optimal non-asymptotic confidence sets for low rank matrix recovery algorithms. These are employed to devise sequential sampling procedures that guarantee recovery of the true matrix in Frobenius norm after a data-driven stopping time \hat{n} for the number of measurements that have to be taken. With high probability, this stopping time is minimax optimal. We detail applications to quantum tomography problems where measurements arise from Pauli observables. We also give a theoretical construction of a confidence set for the density matrix of a quantum state that has optimal diameter in nuclear norm. The non-asymptotic properties of our confidence sets are investigated in a simulation study.

Key words: Low rank recovery, quantum information, confidence sets

1. Introduction

Consider the high-dimensional matrix trace regression model

$$Y_i = \text{tr}(X^i \theta) + \varepsilon_i, \quad i = 1, \dots, n, \quad (1)$$

where the ε_i 's are random noise variables, independent of the random design matrices X^i , and where the matrix θ is the object of inferential interest. We denote the law of (Y, X) given θ by \mathbb{P}_θ . To reflect the structure of the main application we have in mind – quantum tomography, introduced in detail below – we assume that X^i and θ are both $d \times d$ square matrices, and study the case where the number n of measurements taken may be smaller than the effective parameter dimension d^2 . Recovery of θ in such situations is still possible by compressed sensing techniques [5, 22, 21, 29], under two main structural assumptions on the model: 1) the matrix θ is of low rank and 2) the measurement matrices X^i satisfy the restricted isometry (or a related coherence) property. In this case recovery of a rank k matrix θ is possible in Frobenius distance $\|\cdot\|_F$ by, e.g., the Matrix Lasso $\hat{\theta}_n$: for any $\epsilon > 0$ and with high \mathbb{P}_θ -probability,

$$\|\hat{\theta}_n - \theta\|_F < \epsilon \quad \text{as soon as } n \gtrsim kd \log d,$$

where $\overline{\log}d = \log^\eta d, \eta > 0$, is the so-called ‘polylog’ function. The design used in quantum tomography is such that the X^i are randomly drawn from a basis $\{E_1, \dots, E_{d^2}\}$ of the space of $d \times d$ matrices, and one samples fewer than all d^2 basis coefficients $\text{tr}(E_i\theta)$ without losing recovery guarantees for low rank matrices θ . In experimental settings (e.g., [16]), $d = 2^N$ where N is a possibly large number of particles, but θ will represent an approximately pure quantum state, motivating the low rank hypothesis and explaining the interest of quantum information theorists in dimension reduction methods (see the appendix and [14, 13, 25, 10, 15, 32]).

In practice the implementation of the compressed sensing paradigm requires a way to decide how many measurements n should be taken. The preceding theoretical bound $n \gtrsim kd\overline{\log}d$ is not useful for this because it may involve unspecified constants, but also, more importantly, because the rank k of θ is typically not known. Instead one can try to find a *data driven stopping rule* \hat{n} that guarantees that recovery with precision ϵ occurs after \hat{n} measurements, with high probability. In the quantum tomography context such stopping rules are called ‘certificates’ (see Section IV in [10]), as they certify the reconstruction of the true quantum state θ . It is not difficult to see, and will be made precise below, that the construction of such stopping rules is intimately connected to the construction of a (sequential) confidence region for the unknown parameter θ , and due to its importance in applications this topic has received considerable attention recently by physicists, see [8, 3, 33, 2, 10, 31]. None of the previous constructions has succeeded, however, in constructing an *optimal* stopping rule for which $\hat{n} \approx kd\overline{\log}d$ holds with high probability.

The main contribution of the present paper is to construct optimal non-asymptotic Frobenius norm confidence regions for low rank parameters in the model (1), and to use them to devise optimal sequential data driven stopping rules \hat{n} (‘certificates’) for the measurement process. That such procedures exist may at first look surprising in view of negative results in the ‘sparse’ compressed sensing setting in [26], but our results reveal the more favourable information-theoretic structure of the matrix model. While our techniques are based on unbiased risk estimation ideas that were first used in nonparametric statistics (see [24, 30], and also [4]) and that apply in a general setting, we lay out the details for a basic (sub-) Gaussian design and noise model, as well as for the Pauli observation scheme relevant in quantum tomography (see [10] and Condition 1b) below). We shall also address the more difficult question of constructing confidence regions for a quantum state matrix in the stronger nuclear norm. Relationships between our findings and the recent literature on confidence regions for high-dimensional statistical parameters are discussed at the end. We also investigate the performance of our procedures in basic simulation study.

2. The framework of matrix compressed sensing

2.1. Notation

Denote by $\mathbb{M}_d(\mathbb{K})$ the space of $d \times d$ matrices with entries in $\mathbb{K} = \mathbb{C}$ or $\mathbb{K} = \mathbb{R}$. We write $\|\cdot\|_F$ for the usual Frobenius norm on $\mathbb{M}_d(\mathbb{K})$ arising from the inner product $\text{tr}(A^T B) = \langle A, B \rangle_F$. Moreover let $\mathbb{H}_d(\mathbb{K})$ be the set of all Hermitian matrices (equal to the set of all symmetric $d \times d$ matrices when $\mathbb{K} = \mathbb{R}$). The norm symbol $\|\cdot\|$ denotes the standard Euclidean norm on \mathbb{C}^n arising from the Euclidean inner product $\langle \cdot, \cdot \rangle$.

We denote the usual operator norm on $\mathbb{M}_d(\mathbb{K})$ by $\|\cdot\|_{op}$. For $M \in \mathbb{M}_d(\mathbb{K})$ let $(\lambda_k^2 : k = 1, \dots, d)$ be the eigenvalues of $M^T M$ (which are all real-valued and positive). The l_1 -Schatten, *trace*, or *nuclear* norm of M is defined as

$$\|M\|_{S_1} = \sum_{j \leq d} |\lambda_j|.$$

Note that for any matrix M of rank $1 \leq r \leq d$,

$$\|M\|_F \leq \|M\|_{S_1} \leq \sqrt{r} \|M\|_F. \quad (2)$$

We will consider parameter subspaces of $\mathbb{H}_d(\mathbb{K})$ described by low rank constraints on θ , and denote by $R(k)$ the space of all Hermitian $d \times d$ matrices that have rank at most k , $k \leq d$. In quantum tomography applications, we may assume an additional ‘shape constraint’, namely that θ is a density matrix of a quantum state, and hence contained in *state space*

$$\Theta_+ = \{\theta \in \mathbb{H}_d(\mathbb{K}) : \text{tr}(\theta) = 1, \theta \succeq 0\},$$

where $\theta \succeq 0$ means that θ is positive semi-definite. In fact, in most situations, we will only require the bound $\|\theta\|_{S_1} \leq 1$ which holds for any θ in Θ_+ .

2.2. Sensing matrices

We now specify assumptions on the design matrices X^i used in our observation model (1). When θ has real-valued entries we shall restrict to design matrices X^i with real-valued entries too, and for general $\theta \in \mathbb{H}_d(\mathbb{C})$ we shall assume $X^i \in \mathbb{H}_d(\mathbb{C})$. This way, in either case, the measurements $\text{tr}(X_i \theta)$ ’s and hence the Y_i ’s are all real-valued. Note that in Part a) below the design matrices are not Hermitian but our results can easily be generalised to symmetrised sub-Gaussian ensembles (as those considered in ref. [21]). Part b) corresponds to the quantum tomography measurement model used in [13, 25, 10, 14] – we refer to the appendix for a detailed derivation.

Condition 1 a) $\theta \in \mathbb{H}_d(\mathbb{R})$, ‘isotropic’ sub-Gaussian design: The random variables $(X_{m,k}^i)$, $1 \leq m, k \leq d, i = 1, \dots, n$, generating the entries of the random matrix X^i are i.i.d. distributed across all indices i, m, k with

mean zero and unit variance. Moreover, for every $\theta \in \mathbb{M}_d(\mathbb{R})$ such that $\|\theta\|_F \leq 1$ the real random variables $Z_i = \text{tr}(X^i \theta)$ are sub-Gaussian: for some fixed constants $\tau_1, \tau_2 > 0$ independent of θ ,

$$\mathbb{E} e^{\lambda Z_i} \leq \tau_1 e^{\lambda^2 \tau_2^2} \quad \forall \lambda \in \mathbb{R}.$$

- b) $\theta \in \mathbb{H}_d(\mathbb{C})$, **random sampling from a basis ('Pauli design')**: Let $\{E_1, \dots, E_{d^2}\} \subset \mathbb{H}_d(\mathbb{C})$ be a basis of $\mathbb{M}_d(\mathbb{C})$ that is orthonormal for the scalar product $\langle \cdot, \cdot \rangle_F$ and such that the operator norms satisfy, for all $i = 1, \dots, d^2$,

$$\|E_i\|_{op} \leq \frac{K}{\sqrt{d}},$$

for some $K > 0$. [In the Pauli basis case we have $K = 1$.] Assume the X^i , $i = 1, \dots, n$, are draws from the finite family $\mathcal{E} = \{dE_i : i = 1, \dots, d^2\}$ sampled uniformly at random.

The above examples all obey the *matrix restricted isometry property*, that we describe now. Note first that if $\mathcal{X} : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}^n$ is the linear 'sampling' operator

$$\mathcal{X} : \theta \mapsto \mathcal{X}\theta = (\text{tr}(X^1 \theta), \dots, \text{tr}(X^n \theta))^T, \quad (3)$$

so that we can write the model equation (1) as $Y = \mathcal{X}\theta + \varepsilon$, then in the above examples we have the 'expected isometry'

$$\mathbb{E} \frac{1}{n} \|\mathcal{X}\theta\|^2 = \|\theta\|_F^2.$$

Indeed, in the isotropic design case we have

$$\frac{1}{n} \mathbb{E} \|\mathcal{X}\theta\|^2 = \frac{1}{n} \sum_{i=1}^n \mathbb{E} \left(\sum_m \sum_k X_{m,k}^i \theta_{m,k} \right)^2 = \sum_m \sum_k \mathbb{E} X_{m,k}^2 \theta_{m,k}^2 = \|\theta\|_F^2, \quad (4)$$

and in the 'basis case' we have, from Parseval's identity and since the X^i 's are sampled uniformly at random from the basis,

$$\frac{1}{n} \mathbb{E} \|\mathcal{X}\theta\|^2 = \frac{d^2}{n} \sum_{i=1}^n \sum_{j=1}^{d^2} \Pr(X^i = E_j) |\langle E_j, \theta \rangle_F|^2 = \|\theta\|_F^2. \quad (5)$$

The restricted isometry property (RIP) requires that this 'expected isometry' holds, up to constants and with probability $\geq 1 - \delta$, for a given realisation of the sampling operator, and for all $d \times d$ matrices θ of rank at most k :

$$\sup_{\theta \in R(k)} \left| \frac{\frac{1}{n} \|\mathcal{X}\theta\|^2 - \|\theta\|_F^2}{\|\theta\|_F^2} \right| \leq \tau_n(k), \quad (6)$$

where $\tau_n(k)$ are some constants that may depend, among other things, on the rank k and the 'exceptional probability' δ . For the above examples of isotropic and Pauli basis design inequality (6) can be shown to hold with

$$\tau_n^2(k) = c^2 \frac{kd \cdot \overline{\log d}}{n}, \quad (7)$$

where $c = c(\delta) = O(1/\delta^2)$ as $\delta \rightarrow 0$ is a fixed constant. See refs. [5, 25] for these results.

2.3. Gaussian and Bernoulli errors, and Pauli observables

We still have to specify the distribution of the errors ε_i in the model (1). In the quantum tomography setting of Condition 1b), if we fix an element $E_i \in \mathcal{E}$ for the moment, then as detailed in the appendix the observations $Y_i = \text{dtr}(E_i\theta) + \varepsilon_i$ are themselves an average of repeated samples from a Bernoulli random variable B_i taking values $\{1, -1\}$ with probabilities given by

$$\mathbb{P}(B_i = 1) = \frac{1 + \sqrt{\text{dtr}(E_i\theta)}}{2}.$$

More precisely,

$$Y_i = \frac{\sqrt{d}}{T} \sum_{j=1}^T B_{i,j} = d \cdot \text{tr}(E_i\theta) + \varepsilon_i$$

where

$$\varepsilon_i = \frac{\sqrt{d}}{T} \sum_{j=1}^T (B_{i,j} - \mathbb{E}B_{i,j})$$

is the effective error arising from the measurement procedure making use of T preparations to estimate each quantum mechanical expectation value. We could work with this Bernoulli error model directly, but since the ε_i 's are themselves sums of independent random variables, an approximate Gaussian error model will be appropriate, too. Note further that

$$|\varepsilon_i| \leq 2\sqrt{d}, \quad \mathbb{E}\varepsilon_i^2 \leq \frac{d}{T} \text{Var}(B_{i,1}) \leq \frac{d}{T} \quad (8)$$

so the variances $\mathbb{E}\varepsilon_i^2 = \sigma^2$ are bounded by d/T . A natural assumption is then

Condition 2 *The $\varepsilon_i, i = 1, \dots, n$, are i.i.d. $N(0, \sigma^2)$ where $\sigma^2 \leq v$ for some known constant v .*

This unifies the exposition for both designs considered in Condition 1, but we note that our proofs are valid in the exact Bernoulli error model as well, see Remark 2 below.

2.4. Minimax estimation under the RIP

Assuming the matrix RIP from (6) to hold and Gaussian noise $\varepsilon \sim N(0, \sigma^2 I_n)$, one can show that the minimax risk for recovering a Hermitian rank k matrix is

$$\inf_{\hat{\theta}} \sup_{\theta \in R(k)} \mathbb{E}_{\theta} \|\hat{\theta} - \theta\|_F^2 \simeq \sigma^2 \frac{dk}{n}, \quad (9)$$

where \simeq denotes two-sided inequality up to universal constants. For the upper bound one can use the nuclear norm minimisation procedure or matrix Dantzig selector from Candès and Plan [5] (see also [25] for the case of Pauli-design), and needs n to be large enough so that the matrix RIP holds with $\tau_n(k) < c_0$ where c_0 is a small enough numerical constant. Such an estimator $\tilde{\theta}$ then satisfies, for every $\theta \in R(k)$ and those $n \in \mathbb{N}$ for which $\tau_n(k) < c_0$,

$$\|\tilde{\theta} - \theta\|_F^2 \leq D(\delta)\sigma^2 \frac{kd}{n}, \quad (10)$$

with probability $\geq 1 - 2\delta$, and with the constant $D(\delta)$ depending on δ and also on c_0 (suppressed in the notation). Note that the results in [5] use a different scaling in sample size in their Theorem 2.4, but eq. (II.7) in that reference explains that this is just a matter of renormalisation. The same bound holds for the Bernoulli noise model from Subsection 2.3, see [10].

3. Main results

We now turn to the problem of quantifying the uncertainty of estimators $\tilde{\theta}$ that satisfy the risk bound (10). In fact the procedures we construct could be used for any estimator of θ , but the conclusions are most interesting when used for minimax optimal estimators $\hat{\theta}$.

3.1. Confidence sets and sequential sampling protocols

From a statistical point of view the problem at hand is the one of constructing a confidence set for θ : a data-driven subset C_n of $\mathbb{M}_d(\mathbb{C})$ that is ‘centred’ at θ , that satisfies

$$\mathbb{P}_\theta(\theta \in C_n) \geq 1 - \alpha, \quad 0 < \alpha < 1,$$

for a chosen ‘coverage’ or significance level $1 - \alpha$, and such that the Frobenius norm diameter $|C_n|_F$ reflects the accuracy of estimation, that is, it satisfies, with high probability,

$$|C_n|_F^2 \approx \|\tilde{\theta} - \theta\|_F^2.$$

In particular such a confidence set provides, through its diameter $|C_n|_F$, a data-driven estimate of how well the algorithm has recovered the true matrix θ in Frobenius-norm loss, and in this sense provides a quantification of the uncertainty in the estimate.

In an experimental situation confidence sets $(C_n : n \in \mathbb{N})$ can be used to decide sequentially whether more measurements should be taken (to improve the recovery rate), or whether a satisfactory performance has been reached. Concretely, for given n we check if $|C_n|_F \leq \epsilon$, and continue to take further measurements if not. Assuming $\tilde{\theta}$ satisfies the minimax optimal risk bound dk/n from (10), we expect to need, ignoring constants,

$$\frac{dk}{n} < \epsilon^2 \text{ and hence at least } n > \frac{dk}{\epsilon^2}$$

measurements. Note that we also need the RIP to hold with $\tau_n(k)$ from (7) less than a small constant c_0 , which requires the same number of measurements, increased by a further poly-log factor of d (and independently of σ). The goal is then to prove that a sequential procedure based on C_n does *not* require more than approximately

$$n > \frac{dk \overline{\log d}}{\epsilon^2}$$

samples (with high probability). This is made precise in the following definition, where we recall that $R(k)$ denotes the set of $d \times d$ Hermitian matrices of rank at most $k \leq d$.

Definition 1 *Let $\epsilon > 0, \delta > 0$ be given constants. An algorithm \mathcal{A} returning a $d \times d$ matrix $\hat{\theta}$ after $\hat{n} \in \mathbb{N}$ measurements in model (1) is called an (ϵ, δ) - adaptive sampling procedure if, with \mathbb{P}_θ -probability greater than $1 - \delta$, the following properties hold for every $\theta \in R(k)$ and every $1 \leq k \leq d$:*

$$\|\hat{\theta} - \theta\|_F \leq \epsilon, \tag{11}$$

and, for some positive constants $C(\delta), \gamma$, the stopping time \hat{n} satisfies

$$\hat{n} \leq C(\delta) \frac{kd(\log d)^\gamma}{\epsilon^2}. \tag{12}$$

Such an algorithm provides recovery at given accuracy level ϵ with \hat{n} measurements of minimax optimal order of magnitude (up to a poly-log factor), and with probability greater than $1 - \delta$. The sampling algorithm is adaptive since it does not require the knowledge of k , and since the number of measurements required depends only on k and not on the ‘worst case’ rank d .

Our first main result is the following theorem, whose proof relies on the construction of non-asymptotic confidence sets C_n for θ at any sample size n , given in the next subsection.

Theorem 1 *Consider observations in the model (1) under Conditions 1b) and 2, and where $\theta \in \Theta_+$. Then an adaptive sampling algorithm in the sense of Definition 1 exists for any $\epsilon, \delta > 0$.*

The result above holds for isotropic design from Condition 1a) too, without the constraint $\theta \in \Theta_+$, see Remark 1 below. For Pauli design the assumption $\theta \in \Theta_+$ (instead of just $\theta \in \mathbb{M}_d(\mathbb{K})$) is, however, necessary: Else the example of $\theta = 0$ or $\theta = E_i$ – where E_i is an arbitrary element of the Pauli basis – demonstrates that the number of measurements has to be at least of order d^2 : otherwise with positive probability E_i is not drawn at a fixed sample size. On this event both the measurements and $\hat{\theta}$ coincide under the laws \mathbb{P}_0 and \mathbb{P}_{E_i} , so we cannot have $\|\hat{\theta} - 0\|_F < \epsilon$ AND $\|\hat{\theta} - E_i\|_F < \epsilon$ simultaneously for every $\epsilon > 0$, disproving existence of an adaptive sampling algorithm. In fact, the crucial condition for Theorem 1 to work is that the nuclear norms $\|\theta\|_{S_1}$ are bounded by an absolute constant (here = 1), which is violated by $\|E_i\|_{S_1} = \sqrt{d}$.

3.2. Frobenius norm confidence sets based on unbiased risk estimation

3.2.1. An optimal confidence region for $n \leq d^2$

We suppose that we have two samples at hand, the first being used to construct an estimator $\tilde{\theta}$, such as the one from (10). We freeze $\tilde{\theta}$ and the first sample in what follows and all probabilistic statements are under the distribution \mathbb{P}_θ of the second sample Y, X of size $n \in \mathbb{N}$, conditional on the value of $\tilde{\theta}$. We define the following residual sum of squares (RSS) statistic

$$\hat{r}_n = \frac{1}{n} \|Y - \mathcal{X}\tilde{\theta}\|^2 - \sigma^2, \quad (13)$$

which satisfies $\mathbb{E}_\theta \hat{r}_n = \|\theta - \tilde{\theta}\|_F^2$ in the model (1) under Conditions 1 and 2 (see the proof of Theorem 2 below). We assume for now that σ is known, see Subsection 3.2.4 below for a discussion of the necessary modifications in the general case. Given $\alpha > 0$, let $\xi_{\alpha, \sigma}$ be quantile constants such that

$$\Pr \left(\sum_{i=1}^n (\varepsilon_i^2 - 1) > \xi_{\alpha, \sigma} \sqrt{n} \right) = \alpha \quad (14)$$

(these constants converge to the quantiles of a fixed normal distribution as $n \rightarrow \infty$), let $z_\alpha = \log(3/\alpha)$ and, for $z \geq 0$ a fixed constant to be chosen, define the confidence set

$$C_n = \left\{ v \in \mathbb{H}_d(\mathbb{C}) : \|v - \tilde{\theta}\|_F^2 \leq 2 \left(\hat{r}_n + z \frac{d}{n} + \frac{\bar{z} + \xi_{\alpha/3, \sigma}}{\sqrt{n}} \right) \right\}, \quad (15)$$

where

$$\bar{z}^2 = \bar{z}^2(\alpha, d, n, \sigma, v) = z_{\alpha/3} \sigma^2 \max(3\|v - \tilde{\theta}\|_F^2, 4zd/n).$$

Note that in the ‘quantum shape constraint’ case $\theta \in \Theta_+$ we can always upper bound $\|v - \tilde{\theta}\|_F \leq 2$ in the definition of \bar{z} , which gives a confidence set that is easier to compute and of only marginally larger overall diameter. In some situations, however, the quantity \bar{z}/\sqrt{n} is of smaller order than $1/\sqrt{n}$, and the more complicated expression above is generally preferable.

It is not difficult to see (using that $x^2 \lesssim y + x/\sqrt{n}$ implies $x^2 \lesssim y + 1/n$) that the mean square Frobenius norm diameter of C_n is of order

$$\mathbb{E}_\theta |C_n|_F^2 \lesssim \|\tilde{\theta} - \theta\|_F^2 + \frac{zd + z_{\alpha/3}}{n} + \frac{\xi_{\alpha/3, \sigma}}{\sqrt{n}}. \quad (16)$$

Whenever $d \geq \sqrt{n}$ – so as long as at most $n \leq d^2$ measurements have been taken – the deviation terms are of smaller order than kd/n for any $k \geq 1$, and hence C_n has minimax optimal expected squared diameter whenever the estimator $\tilde{\theta}$ is minimax optimal as in (10).

The following result shows that C_n is a valid confidence set for arbitrary Hermitian $d \times d$ matrices (without any rank constraint). Note that the result is non-asymptotic – it holds for every $n \in \mathbb{N}$.

Theorem 2 Let $\theta \in \mathbb{H}_d(\mathbb{C})$ be arbitrary and let \mathbb{P}_θ be the distribution of Y, X from model (1) under Condition 2.

a) Assume the design satisfies Condition 1a) and let C_n be given by (15) with $z = 0$. We then have for every $n \in \mathbb{N}$ that

$$\mathbb{P}_\theta(\theta \in C_n) \geq 1 - \frac{2\alpha}{3} - 2e^{-cn}$$

where c is a numerical constant. In the case of standard Gaussian design, $c = 1/24$ is admissible.

b) Assume the design satisfies Condition 1b) with constant $K > 0$, let C_n be given by (15) with $z > 0$ and assume also that $\theta \in \Theta_+$ and $\tilde{\theta} \in \Theta_+$ (that is, both satisfy the ‘quantum shape constraint’). Then for every $n \in \mathbb{N}$,

$$\mathbb{P}_\theta(\theta \in C_n) \geq 1 - \frac{2\alpha}{3} - 2e^{-C(K)z}$$

where $C(K) = 1/[(16 + 8/3)K^2]$.

In Part a), if we want to control the coverage probability at level $1 - \alpha$, n needs to be large enough so that the third deviation term is controlled at level $\alpha/3$. In the Gaussian design case with $\alpha = 0.05$, $n \geq 100$ is sufficient, for smaller sample sizes one can use the confidence region from the next subsection. The bound in b) is entirely non-asymptotic for suitable choices of z . Also note that the quantile constants z, z_α, ξ_α all scale at least as $O(\log(1/\alpha))$ in the desired coverage level $\alpha \rightarrow 0$.

As mentioned above, the confidence set from Theorem 2 is optimal whenever the desired performance of $\|\theta - \tilde{\theta}\|_F^2$ is no better than of order $1/\sqrt{n}$, corresponding to the important regime $n \leq d^2$ for sequential sampling algorithms. Refinements for measurement scales $n \geq d^2$ are also of interest - we present two optimal approaches in the next two subsections for the designs from Condition 1.

3.2.2. Isotropic design and a confidence set based on U -statistics

Consider isotropic i.i.d design from Condition 1a), and an estimator $\tilde{\theta}$ based on an initial sample of size n (all statements that follow are conditional on that sample). Collect another n samples to perform the uncertainty quantification step. Define the U -statistic

$$\hat{R}_n = \frac{2}{n(n-1)} \sum_{i < j} \sum_{m,k} (Y_i X_{m,k}^i - \tilde{\theta}_{m,k})(Y_j X_{m,k}^j - \tilde{\theta}_{m,k}) \quad (17)$$

whose \mathbb{E}_θ -expectation, conditional on $\tilde{\theta}$, equals $\|\theta - \tilde{\theta}\|_F^2$ in view of

$$\mathbb{E} Y_i X_{m,k}^i = \mathbb{E} \sum_{m',k'} X_{m',k'}^i X_{m,k}^i \theta_{m',k'} = \theta_{m,k}.$$

Define

$$C_n = \left\{ v \in \mathbb{H}_d(\mathbb{R}) : \|v - \tilde{\theta}\|_F^2 \leq \hat{R}_n + z_{\alpha,n} \right\} \quad (18)$$

where

$$z_{\alpha,n} = \frac{C_1 \|\theta - \tilde{\theta}\|_F}{\sqrt{n}} + \frac{C_2 d}{n}$$

and $C_1 \geq \zeta_1 \|\theta\|_F$, $C_2 \geq \zeta_2 \|\theta\|_F^2$ with ζ_i constants depending on α and the upper bound v for σ from Condition 2. Note that if $\theta \in \Theta_+$ then $\|\theta\|_F \leq 1$ can be used as an upper bound in C_i , $i = 1, 2$. In practice the constants ζ_i can be calibrated by Monte Carlo simulations (see the implementation section below), or chosen based on concentration inequalities for U -statistics (see ref. [12], Theorem 4.4.8). This confidence set has expected diameter

$$\mathbb{E}_\theta |C_n|_F^2 \lesssim \|\tilde{\theta} - \theta\|_F^2 + \frac{C_1 + C_2 d}{n},$$

and hence is compatible with any minimax recovery rate $\|\tilde{\theta} - \theta\|_F^2 \lesssim kd/n$ from (10), where $k \geq 1$ is now arbitrary. For suitable choices of ζ_i we now show that C_n also has non-asymptotic coverage.

Theorem 3 *Assume Conditions 1a) and 2, and let C_n be as in (18). For every $\alpha > 0$ we can choose $\zeta_i(\alpha) = O(\sqrt{1/\alpha})$, $i = 1, 2$, large enough so that for every $n \in \mathbb{N}$ we have*

$$\mathbb{P}_\theta(\theta \in C_n) \geq 1 - \alpha.$$

3.2.3. Pauli design: Re-averaging basis elements when $n \geq d^2$

For the design from Condition 1b) where we sample uniformly at random from a (scaled) basis $\{dE_1, \dots, dE_{d^2}\}$ of $\mathbb{M}_d(\mathbb{C})$, the U -statistic approach from Theorem 3 appears not to be viable, and thus for $d \leq \sqrt{n}$ the existence of an optimal confidence region still needs to be ensured. When $d \leq \sqrt{n}$ we are taking $n \geq d^2$ measurements, and there is no need to sample at *random* from the basis as we can measure each individual coefficient, possibly even multiple times. Repeatedly sampling a basis coefficient $\text{tr}(E_k \theta)$ leads to a reduction of the variance of the measurement by averaging. More precisely, when taking $n = md^2$ measurements for some (for simplicity integer) $m \geq 1$, and if $(Y_{k,l} : l = 1, \dots, m)$ are the measurements Y_i corresponding to the basis element E_k , $k \in \{1, \dots, d^2\}$, we can form averaged measurements

$$Z_k = \frac{1}{\sqrt{m}} \sum_{l=1}^m Y_{k,l} = \sqrt{m} d \langle E_k, \theta \rangle_F + \epsilon_k, \quad \epsilon_k = \frac{1}{\sqrt{m}} \sum_{l=1}^m \varepsilon_l \sim N(0, \sigma^2).$$

We can then define the new measurement vector $\tilde{Z} = (\tilde{Z}_1, \dots, \tilde{Z}_{d^2})^T$ (using also $m = n/d^2$)

$$\tilde{Z}_k = Z_k - \sqrt{n} \langle \tilde{\theta}, E_k \rangle = \sqrt{n} \langle E_k, \theta - \tilde{\theta} \rangle_F + \epsilon_k, \quad k = 1, \dots, d^2$$

and the statistic

$$\hat{R}_n = \frac{1}{n} \|\tilde{Z}\|_{\mathbb{R}^{d^2}}^2 - \frac{\sigma^2 d^2}{n} \quad (19)$$

which estimates $\|\theta - \tilde{\theta}\|_F^2$ with precision

$$\begin{aligned} \hat{R}_n - \|\theta - \tilde{\theta}\|_F^2 &= \frac{2}{\sqrt{n}} \sum_{k=1}^{d^2} \epsilon_k \langle E_k, \theta - \tilde{\theta} \rangle_F + \frac{1}{n} \sum_{k=1}^{d^2} (\epsilon_k^2 - \mathbb{E}\epsilon^2) \\ &= O_P \left(\frac{\sigma \|\theta - \tilde{\theta}\|_F}{\sqrt{n}} + \frac{\sigma^2 d}{n} \right). \end{aligned}$$

Hence, for z_α the quantiles of a $N(0, 1)$ distribution and $\xi_{\alpha, \sigma}$ as in (14) with d^2 replacing n there, we can define a confidence set

$$\bar{C}_n = \left\{ v \in \mathbb{H}_d(\mathbb{C}) : \|v - \tilde{\theta}\|_F^2 \leq \hat{R}_n + \frac{z_{\alpha/2} \sigma \|\theta - \tilde{\theta}\|_F}{\sqrt{n}} + \frac{\xi_{\alpha/2, \sigma} d}{n} \right\} \quad (20)$$

which has non-asymptotic coverage

$$\mathbb{P}_\theta(\theta \in \bar{C}_n) \geq 1 - \alpha$$

for every $n \in \mathbb{N}$, by similar (in fact, since Lemma 1 is not needed, simpler) arguments as in the proof of Theorem 2 below. The expected diameter of \bar{C}_n is by construction

$$\mathbb{E}_\theta |\bar{C}_n|_F^2 \lesssim \|\theta - \tilde{\theta}\|_F^2 + \frac{\sigma^2 d}{n}, \quad (21)$$

now compatible with *any* rate of recovery kd/n , $1 \leq k \leq d$. The case of unknown variance is discussed in the next subsection.

3.2.4. Unknown variance

The U -statistic based confidence set from (18) does not require knowledge of σ but works only for the design from Condition 1a). For Pauli design from Condition 1b) we can use the confidence sets C_n in Theorem 2 or \bar{C}_n in (20), but these do require exact knowledge of the noise variance σ^2 . As described before (8) above, in the Pauli case σ^2 can be a priori bounded by d/T , where T is the number of preparations used to measure each individual Pauli observable. If $T \geq n$ then the statistics \hat{r}_n and \hat{R}_n from (13) and (19) above can be used without subtracting σ^2 and $\sigma^2 d^2/n$, respectively, in their definitions. The coverage proofs then go through with minor modifications simply by noting that these centerings are of sufficiently small order of magnitude $\sigma^2 \leq d/T \leq d/n$ and $\sigma^2 d^2/n \leq d^3/Tn \leq d/n$ compared to the minimax rate of estimation, and by using the upper bound $\sigma^2 \leq v = d/T$ in all relevant constants featuring in the definition of C_n, \bar{C}_n .

Typically preparing $T \geq n$ measurements of a fixed Pauli observable is not a major problem in experimental situations. If for some reason this cannot be

done, one can make sure that each $\text{tr}(E_i\theta)$ is at least measured twice (so $T \geq 2$), say in batches $Y_1, \dots, Y_{n/2}$ and $Y_{n/2+1}, \dots, Y_n$, and then use the modified statistic

$$\tilde{r}_n = \frac{2}{n} \sum_{i=1}^{n/2} (Y_i - \langle X^i, \tilde{\theta} \rangle_F) (Y_{i+n/2} - \langle X^i, \tilde{\theta} \rangle_F)$$

in the construction of the confidence set. Arguments similar to above, using concentration inequalities for Gaussian chaos of order two (Theorem 3.1.9 in [12]) then allow for the construction of a confidence region that does neither require knowledge of $\sigma^2 \leq v$ nor $T \geq n$. Details are omitted.

3.3. A confidence set in trace norm under quantum shape constraints

The confidence sets from the previous subsections are all valid in the sense that they contain information about the recovery of θ by $\tilde{\theta}$ in Frobenius norm $\|\cdot\|_F$. It is of interest to obtain results in stronger norms, such as for instance the nuclear norm $\|\cdot\|_{S_1}$, which is particularly meaningful for quantum tomography problems since it then corresponds to the total variation distance on the set of ‘probability density matrices’. The absence of the ‘Hilbert space geometry’ induced by the relationship of the Frobenius norm to the inner product $\langle \cdot, \cdot \rangle_F$ makes this problem significantly harder, both technically and from an information-theoretic point of view. In particular the quantum shape constraint $\theta \in \Theta_+$ is crucial to obtain any results whatsoever. For the theoretical results presented here it will be more convenient to perform an asymptotic analysis where $\min(n, d) \rightarrow \infty$ (with o, O -notation to be understood accordingly).

Instead of Condition 1 we now consider more generally any design $(X^i, i = 1, \dots, n)$ in model (1) that satisfies the matrix RIP (6) with

$$\tau_n(k) = c \sqrt{kd \frac{\log(d)}{n}}. \quad (22)$$

We shall still use the convention discussed before Condition 1 that θ and the matrices X^i are such that $\text{tr}(X^i\theta)$ is always real-valued.

In contrast to the results from the previous section we shall now assume a minimal low rank constraint on the parameter space:

Condition 3 $\theta \in R^+(k) := R(k) \cap \Theta_+$ for some k satisfying

$$k \sqrt{\frac{d \log d}{n}} = o(1),$$

This in particular implies that the RIP holds with $\tau_n(k) = o(1)$. Given this minimal rank constraint $\theta \in R^+(k)$, we now show that it is possible to construct a confidence set C_n that adapts to any low rank $1 \leq k_0 < k$. Here we may choose $k = d$ but note that this forces $n \gg d^2$ (for Condition 3 to hold with $k = d$).

We assume that there exists an estimator $\tilde{\theta}_{\text{Pilot}}$ that satisfies, uniformly in $R(k_0)$ for any $k_0 \leq k$ and for n large enough,

$$\|\tilde{\theta}_{\text{Pilot}} - \theta\|_F^2 \leq D\sigma^2 \frac{k_0 d}{n} := \frac{r_n^2(k_0)}{4} \quad (23)$$

where $D = D(\delta)$ depends on δ , and where so-defined r_n will be used frequently below. Such estimators exist as has already been discussed before (10). We shall in fact require a little more, namely the following oracle inequality: for any k and any matrix S of rank $k \leq d$, with high probability and for n large enough,

$$\|\tilde{\theta}_{\text{Pilot}} - \theta\|_F \lesssim \|\theta - S\|_F + r_n(k), \quad (24)$$

which implies (23). Such inequalities exist assuming the RIP and Condition 3, see, e.g., Theorem 2.8 in ref. [5]. Starting from $\tilde{\theta}_{\text{Pilot}}$ one can construct (see Theorem 5 below) an estimator that recovers $\theta \in R(k)$ in nuclear norm at rate $k\sqrt{d/n}$, which is again optimal from a minimax point of view, even under the quantum constraint (as discussed, e.g., in ref. [21]). We now construct an adaptive confidence set for θ centred at a suitable projection of $\tilde{\theta}_{\text{Pilot}}$ onto Θ_+ .

In the proof of Theorem 4 below we will construct estimated eigenvalues $(\hat{\lambda}_j, j = 1, \dots, d)$ of θ (see after Lemma 3). Given those eigenvalues and $\tilde{\theta}_{\text{Pilot}}$, we choose \hat{k} to equal the smallest integer $\leq d$ such that there exists a rank \hat{k} matrix $\tilde{\theta}'$ for which

$$\|\tilde{\theta}' - \tilde{\theta}_{\text{Pilot}}\|_F \leq r_n(\hat{k}) \text{ and } 1 - \sum_{J \leq \hat{k}} \hat{\lambda}_J \leq 2\hat{k}\sqrt{d/n}$$

is satisfied. Such \hat{k} exists with high probability (since the inequalities are satisfied for the true θ and λ_j 's, as our proofs imply). Define next \hat{v} to be the $\langle \cdot, \cdot \rangle_F$ -projection of $\tilde{\theta}_{\text{Pilot}}$ onto

$$R^+(2\hat{k}) := R(2\hat{k}) \cap \Theta_+$$

and note that, since $2\hat{k} \geq \hat{k}$,

$$\|\tilde{\theta}_{\text{Pilot}} - \hat{v}\|_F = \|\tilde{\theta}_{\text{Pilot}} - R^+(2\hat{k})\|_F \leq \|\tilde{\theta}_{\text{Pilot}} - \tilde{\theta}'\|_F \leq r_n(\hat{k}). \quad (25)$$

Finally define, for C a constant chosen below,

$$C_n = \left\{ v \in \Theta_+ : \|v - \hat{v}\|_{S_1} \leq C\sqrt{\hat{k}}r_n(\hat{k}) \right\}. \quad (26)$$

Theorem 4 *Assume Condition 3 for some $1 \leq k \leq d$, and let $\delta > 0$ be given. Assume that with probability greater than $1 - 2\delta/3$, a) the RIP (6) holds with $\tau_n(k)$ as in (22) and b) there exists an estimator $\tilde{\theta}_{\text{Pilot}}$ for which (24) holds. Then we can choose $C = C(\delta)$ large enough so that, for C_n as in the last display,*

$$\liminf_{\min(n,d) \rightarrow \infty} \inf_{\theta \in R^+(k)} \mathbb{P}_\theta(\theta \in C_n) \geq 1 - \delta.$$

Moreover, uniformly in $R^+(k_0)$, $1 \leq k_0 \leq k$, and with \mathbb{P}_θ -probability greater than $1 - \delta$,

$$|\mathcal{C}_n|_{S_1} \lesssim \sqrt{k_0} r_n(k_0).$$

Theorem 4 shows how the quantum shape constraint allows for the construction of an optimal nuclear norm confidence set that adapts to the unknown low rank structure. A careful study of certain hypothesis testing problems (combined with lower bound techniques for confidence sets as in [17, 26]) shows that the assumption $\theta \in R^+(k)$ in the above theorem is actually necessary, and cannot be relaxed to $\theta \in R(k)$. See [7], Theorem 4.

3.4. Conclusions

We have constructed adaptive confidence regions for matrix parameters θ in the trace regression model (1). These confidence regions contract at the minimax optimal rates for low rank parameters, either in Frobenius or nuclear norm, and are ‘honest’ (in the sense of [24], see also [30, 17]). The conditions employed are naturally compatible with quantum tomography applications - where θ is the density matrix of a quantum state, and where the noise variance has an a priori upper bound that can be controlled experimentally. This in turn can be used to demonstrate the existence of fully adaptive sequential sampling protocols that generate valid certificates for the recovery of unknown low rank quantum states.

While it can be shown on the one hand (see Theorem 4 in [7]) that our results for the nuclear norm (Theorem 4) fundamentally rely on the ‘quantum shape constraint’ $\theta \in \Theta_+$, our results for the Frobenius norm on the other hand are valid in a general compressed sensing inference setting. This may seem surprising in light of negative results in [26], where it is shown that in the related ‘sparse’ high-dimensional linear model, signal strength assumptions (inspired by the nonparametric statistics literature, [11, 17]) are generally necessary for the existence of ℓ_2 -confidence regions for the entire parameter vector. However, the information theoretic structure of the matrix inference problem is different, as is also illustrated by the fact that the signal detection rates in the model (1) in Frobenius norm do *not* depend on the low rank structure at all (see Theorem 1 in [7]). In this sense, our findings in the matrix regression model form a remarkable exception to the rule that uncertainty quantification methodology does not generally exist for high-dimensional adaptive algorithms, unless one restricts the inferential interest to a simple semi-parametric low-dimensional functional ([34, 35, 20, 6]).

4. Simulation experiments

In order to illustrate the methods from this paper, we present some numerical simulations. The setting of the experiments is as follows: A random matrix $\eta \in \mathbb{M}_d(\mathbb{C})$ of norm $\|\eta\|_F = R^{1/2}$ is generated according to two distinct procedures that we will specify later, and the observations are now

$$\bar{Y}_i = \text{tr}(X^i \eta) + \varepsilon_i.$$

where the ε_i are i.i.d. Gaussian of mean 0 and variance 1. The observations are reparametrised so that η represents the ‘estimation error’ $\theta - \hat{\theta}$, and we investigate how well the statistics

$$\hat{r}_n = \frac{1}{n} \|\bar{Y}\| - 1 \text{ and } \hat{R}_n = \frac{2}{n(n-1)} \sum_{i < j} \sum_{m,k} \bar{Y}_i X_{m,k}^i \bar{Y}_j X_{m,k}^j$$

estimate the ‘accuracy of estimation’ $\|\eta\|_F^2 = \|\theta - \hat{\theta}\|_F^2$, conditional on the value of $\hat{\theta}$. We will choose η in order to illustrate two extreme cases: a first one where the nuclear norm $\|\eta\|_{S_1}$ is ‘small’, corresponding to a situation where the quantum constraint is fulfilled; and a second one where the nuclear norm is large, corresponding to a situation where the quantum constraint is *not* fulfilled. More precisely we generate the parameter η in two ways:

- ‘Random Dirac’ case: set a single entry (with position chosen at random on the diagonal) of η to $R^{1/2}$, and all the other coordinates equal to 0.
- ‘Random Pauli’ case: Set η equal to a Pauli basis element chosen uniformly at random and then multiplied by $R^{1/2}$.

The designs that we consider are the Gaussian design, and the Pauli design, described in Condition 1. We perform experiments with $d = 32$, $R \in \{0.1, 1\}$ and $n \in \{100, 200, 500, 1000, 2000, 5000\}$. Note that $d^2 = 1024$, so that the first four choices of n correspond to the important regime $n < d^2$. Our results are plotted as a function of the number n of samples in Figures 1, 2, 3, 4. The solid red and blue curves are the median errors of the normalised estimation errors

$$\frac{\sqrt{\hat{R}_n - R}}{R^{1/2}}, \quad \text{and} \quad \frac{\sqrt{\hat{r}_n - R}}{R^{1/2}},$$

after 1000 iterations, and the dotted lines are respectively, the (two-sided) 90% quantiles. We also report (see Tables 1, 2, 3, 4) how well the confidence sets based on these estimates of the norm perform in terms of coverage probabilities, and of diameters. The diameters are computed as

$$\left(\hat{R}_n + \frac{C_{\text{UStat}} d}{n} + \frac{C'_{\text{UStat}} \hat{R}_n^{1/2}}{\sqrt{n}} \right)^{1/2},$$

for the U-Statistic approach and

$$\left(\hat{r}_n + \frac{C_{\text{RSS}}}{\sqrt{n}} + \frac{C'_{\text{RSS}} \hat{r}_n^{1/2}}{\sqrt{n}} \right)^{1/2},$$

for the RSS approach, where we have chosen $C_{\text{UStat}} = 2.5$, $C_{\text{RSS}} = 1$ and $C'_{\text{UStat}} = C_{\text{RSS}} = 6$ for all experiments –calibrated to a 95% coverage level. From these numerical results, several observations can be made:

- 1) In Gaussian random designs, the results are insensitive to the nature of η (see Figures 1 and 2 and Tables 1 and 2). This is not surprising since the Gaussian design is ‘isotropic’.

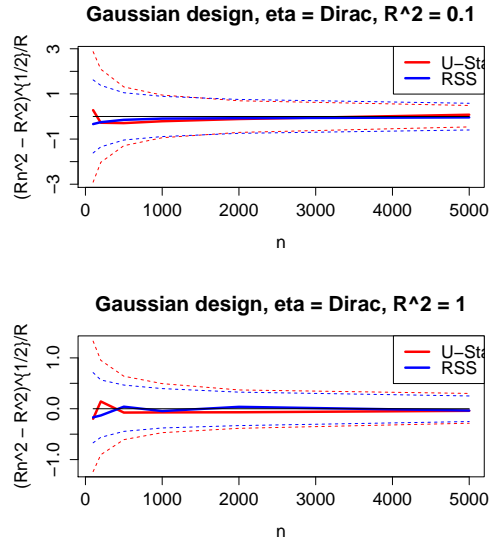


FIG 1. Gaussian design, and random Dirac (a single entry, chosen at random, is non-zero on the diagonal) η , with $R = 0.1$ (left picture) and $R = 1$ (right picture).

2) For Pauli designs with the quantum constraint (see Figure 3 and Table 3) the RSS method works quite well even for small sample sizes. But the U-Stat method is not very reliable – indeed we see no empirical evidence that Theorem 3 should also hold true for Pauli design.

3) For Pauli design and when the quantum shape constraint is *not* satisfied our methods cease to provide reliable results (see Figure 4 and in particular Table 4). Indeed, when the matrix η is chosen itself as a random Pauli (which is the hardest signal to detect under Pauli design) both the RSS and the U-Stat approach perform poorly. The confidence set are not honest anymore, which is in line with the theoretical limitations we observe in Theorem 2. Figure 4 illustrates that the methods do not detect the signal, since the norm of η is largely undervalued for small sample sizes. These limitations are less pronounced when $n \geq d^2$. In this case one could use alternatively the re-averaging approach from Subsection 3.2.3 (not investigated in the simulations) to obtain honest results without the quantum shape constraint.

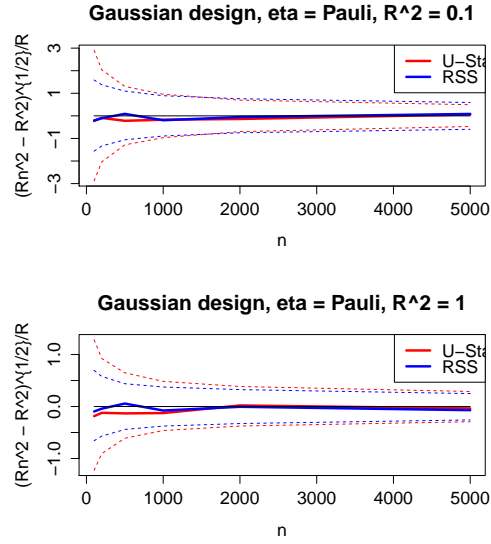


FIG 2. Gaussian design, and random Pauli η , with $R = 0.1$ (left picture) and $R = 1$ (right picture).

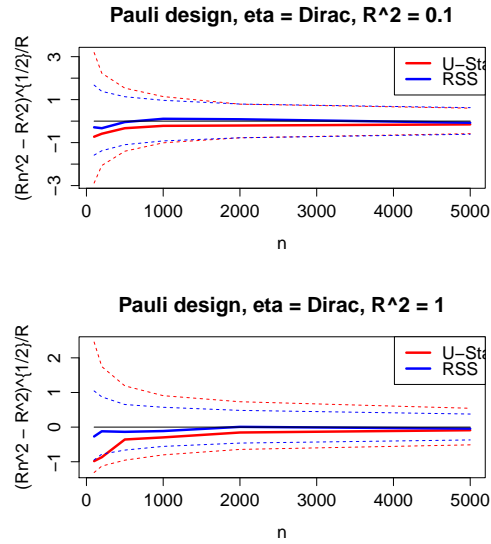


FIG 3. Pauli design, and random Dirac (a single entry, chosen at random, is non-zero on the diagonal) η , with $R = 0.1$ (left picture) and $R = 1$ (right picture).

	$R = 0.1$						$R = 1$					
n	100	200	500	1000	2000	5000	100	200	500	1000	2000	5000
Coverage U-Stat	0.97	0.98	0.99	1.00	1.00	1.00	0.93	0.96	0.97	0.98	0.98	0.98
Diameter U-Stat	1.10	0.64	0.34	0.24	0.18	0.14	2.43	1.84	1.44	1.27	1.17	1.10
Coverage RSS	0.97	0.97	0.98	0.98	0.98	0.98	0.99	0.99	0.99	0.99	0.99	0.99
Diameter RSS	0.38	0.31	0.23	0.19	0.16	0.14	1.69	1.49	1.32	1.22	1.16	1.10

TABLE 1
Gaussian design, and random Dirac (a single entry, chosen at random, is non-zero on the diagonal) η , with $R = 0.1$ (left table) and $R = 1$ (right table).

	$R = 0.1$						$R = 1$					
n	100	200	500	1000	2000	5000	100	200	500	1000	2000	5000
Coverage U-Stat	0.98	0.98	0.99	0.99	1.0	1.0	0.93	0.95	0.97	0.98	0.98	0.98
Diameter U-Stat	1.10	0.62	0.34	0.24	0.18	0.14	2.40	1.83	1.43	1.27	1.18	1.10
Coverage RSS	0.98	0.98	0.97	0.97	0.97	0.97	0.99	0.99	0.99	0.99	1.00	1.00
Diameter RSS	0.39	0.31	0.23	0.19	0.17	0.14	1.71	1.49	1.31	1.22	1.16	1.10

TABLE 2
Gaussian design, and random Pauli η , with $R = 0.1$ (left table) and $R = 1$ (right table).

5. Proofs

5.1. Proof of Theorem 1

Before we define the algorithm and prove the result, a few preparatory remarks are required: Our sequential procedure will be implemented in $m = 1, 2, \dots, T$ potential steps, in each of which $2 \cdot 2^m = 2^{m+1}$ measurements are taken. The arguments below will show that we can restrict the search to at most

$$T = O(\log(d/\epsilon))$$

steps. We also note that from the discussion after (6) – in particular since $c = c(\delta)$ from (7) is $O(1/\delta^2)$ – a simple union bound over $m \leq T$ implies that the RIP holds with probability $\geq 1 - \delta'$, some $\delta' > 0$, *simultaneously* for every $m \leq T$ satisfying $2^m \geq c'kd\log d$, and with $\tau_{2^m}(k) < c_0$, where c' is a constant that depends on δ', c_0 only. The maximum over $T = O(\log(d/\epsilon))$ terms is absorbed in a slightly enlarged poly-log term. Hence, simultaneously for all such sample sizes $2^m, m \leq T$, a nuclear norm regulariser exists that achieves the optimal rate from (10) with $n = 2^m$ and for every $k \leq d$, with probability greater than $1 - \delta/3$. Projecting this estimator onto Θ_+ changes the Frobenius error only by a universal multiplicative constant (arguing as in (25) below), and we denote by $\tilde{\theta}_{2^m} \in \Theta_+$ the resulting estimator computed from a sample of size 2^m .

We now describe the algorithm at the m -th step: Split the 2^{m+1} observations into two halves and use the first subsample to construct $\tilde{\theta}_{2^m} \in \Theta_+$ satisfying (10) with \mathbb{P}_θ -probability $\geq 1 - \delta/3$. Then use the other 2^m observations to construct a confidence set C_{2^m} for θ centred at $\tilde{\theta}_{2^m}$: if $2^m < d^2$ we take C_{2^m} from (15) and

	$R = 0.1$						$R = 1$					
n	100	200	500	1000	2000	5000	100	200	500	1000	2000	5000
Coverage U-Stat	0.97	0.98	0.98	0.99	0.98	0.98	0.85	0.54	0.69	0.69	0.70	0.71
Diameter U-Stat	1.10	0.63	0.34	0.24	0.18	0.14	2.28	1.87	1.43	1.26	1.18	1.10
Coverage RSS	0.96	0.96	0.96	0.96	0.97	0.97	0.88	0.89	0.88	0.88	0.88	0.88
Diameter RSS	0.39	0.29	0.23	0.19	0.16	0.14	1.70	1.50	1.30	1.21	1.16	1.10

TABLE 3
 Pauli design, and random Dirac (a single entry, chosen at random, is non-zero on the diagonal) η , with $R = 0.1$ (left table) and $R = 1$ (right table).

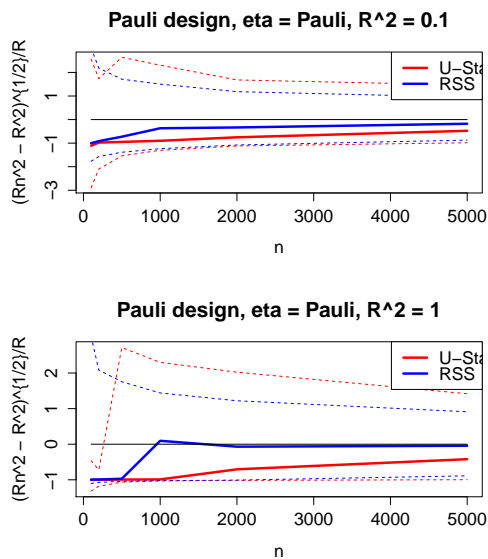


FIG 4. Pauli design, and random Pauli η , with $R = 0.1$ (left picture) and $R = 1$ (right picture).

if $2^m \geq d^2$ we take C_{2^m} from (20) – in both cases of non-asymptotic coverage at least $1 - \alpha$, $\alpha = \delta/(3T)$ [If σ is unknown we proceed as described in Subsection 3.2.4]. If $|C_{2^m}|_F \leq \epsilon$ we terminate the procedure ($m = \hat{m}$, $\hat{n} = 2^{\hat{m}+1}$, $\hat{\theta} = \hat{\theta}_{2^{\hat{m}}}$), but if $|C_{2^m}|_F > \epsilon$ we repeat the above procedure with $2 \cdot 2^{m+1} = 2^{m+1+1}$ new measurements, etc., until the algorithm terminates, in which case we have used

$$\sum_{m \leq \hat{m}} 2^{m+1} \lesssim 2^{\hat{m}} \approx \hat{n}$$

measurements in total.

To analyse this algorithm, recall that the quantile constants z, z_α, ξ_α appearing in the confidence sets (15) and (20) for our choice of $\alpha = \delta/(3T)$ grow at most as $O(\log(1/\alpha)) = O(\log T) = o(\log d)$. In particular in view of (10) and (16) or (21) the algorithm necessarily stops at a ‘maximal sample size’ $n = 2^{T+1}$

	$R = 0.1$						$R = 1$					
n	100	200	500	1000	2000	5000	100	200	500	1000	2000	5000
Coverage U-Stat	0.97	0.97	0.96	0.86	0.65	0.58	0.82	0.22	0.25	0.27	0.30	0.37
Diameter U-Stat	1.09	0.57	0.34	0.25	0.18	0.15	2.45	2.09	1.33	1.38	1.19	1.09
Coverage RSS	0.93	0.86	0.77	0.77	0.77	0.77	0.12	0.19	0.40	0.63	0.56	0.53
Diameter RSS	0.38	0.29	0.22	0.19	0.16	0.14	1.71	1.56	1.31	1.26	1.14	1.08

TABLE 4
Pauli design, and random Pauli η , with $R = 0.1$ (left table) and $R = 1$ (right table).

in which the squared Frobenius risk of the maximal model ($k = d$) is controlled at level ϵ . Such $T \in \mathbb{N}$ is $O(\log(d/\epsilon))$ and depends on $\sigma, d, \epsilon, \delta$, hence can be chosen by the experimenter.

To prove that this algorithms works we show that the event

$$\left\{ \|\hat{\theta} - \theta\|_F^2 > \epsilon^2 \right\} \cup \left\{ \hat{n} > \frac{C(\delta)kd(\log d)^\gamma}{\epsilon^2} \right\} = A_1 \cup A_2$$

has probability at most $2\delta/3$ for large enough $C(\delta), \gamma$. By the union bound it suffices to bound the probability of each event separately by $\delta/3$. For the first: Since \hat{n} has been selected we know $|C_{\hat{n}}|_F \leq \epsilon$ and since $\hat{\theta} = \theta_{\hat{n}}$ the event A_1 can only happen when $\theta \notin C_{\hat{n}}$. Therefore

$$\mathbb{P}_\theta(A_1) \leq \mathbb{P}_\theta(\theta \notin C_{\hat{n}}) \leq \sum_{m=1}^T \mathbb{P}_\theta(\theta \notin C_{2^m}) \leq \delta \frac{T}{3T} = \frac{\delta}{3}.$$

For A_2 , whenever $\theta \in R(k)$ and for all $m \leq T$ for which $2^m \geq c'kd\overline{\log d}$, we have, as discussed above, from (16) or (21) and (10) that

$$\mathbb{E}_\theta |C_{2^m}|_F^2 \leq D' \frac{kd \log T}{2^m},$$

where D' is a constant. In the last inequality the expectation is taken under the distribution of the sample used for the construction of C_{2^m} , and it holds on the event on which $\tilde{\theta}_{2^m}$ realises the risk bound (10). Then let $C(\delta), \gamma$ be large enough so that $C(\delta)kd(\log d)^\gamma/\epsilon^2 \geq c'kd\overline{\log d}$ and let $m_0 \in \mathbb{N}$ be the smallest integer such that

$$2^{m_0} > \frac{C(\delta)kd(\log d)^\gamma}{\epsilon^2}.$$

Then, for $C(\delta)$ large enough and since $T = O(\log(d/\epsilon))$,

$$\mathbb{P}_\theta \left(\hat{n} > \frac{C(\delta)kd(\log d)^\gamma}{\epsilon^2} \right) \leq \mathbb{P}_\theta (|C_{2^{m_0}}|_F^2 > \epsilon^2) \leq \frac{\mathbb{E}_\theta |C_{2^{m_0}}|_F^2}{\epsilon^2} \leq \frac{D' \log T}{C(\delta)(\log d)^\gamma} < \delta/3,$$

by Markov's inequality, completing the proof.

Remark 1 (Isotropic sampling) The proof above works for isotropic design from Condition 1a) likewise. When $2^m \geq d^2$ we replace the confidence set (20) in

the above proof by the confidence set from (18). Assuming also that $\|\theta\|_F \leq M$ for some fixed constant M we can construct a similar upper bound for T and the above proof applies directly (with T of slighter larger but still small enough order).

5.2. Proof of Theorem 2

By Lemma 1 below with $\vartheta = \tilde{\theta} - \theta$ the \mathbb{P}_θ -probability of the complement of the event

$$\mathcal{E} = \left\{ \left| \frac{1}{n} \|\mathcal{X}(\tilde{\theta} - \theta)\|^2 - \|\tilde{\theta} - \theta\|_F^2 \right| \leq \max \left(\frac{\|\theta - \tilde{\theta}\|_F^2}{2}, \frac{zd}{n} \right) \right\}$$

is bounded by the deviation terms $2e^{-cn}$ and $2e^{-C(K)z}$, respectively (note $z = 0$ in Case a)). We restrict to this event in what follows. We can decompose

$$\hat{r}_n = \frac{1}{n} \|\mathcal{X}(\tilde{\theta} - \theta)\|^2 + \frac{2}{n} \langle \varepsilon, \mathcal{X}(\theta - \tilde{\theta}) \rangle + \frac{1}{n} \sum_{i=1}^n (\varepsilon_i^2 - \mathbb{E}\varepsilon_i^2) = A + B + C.$$

Since $\mathbb{P}(Y + Z < 0) \leq \mathbb{P}(Y < 0) + \mathbb{P}(Z < 0)$ for any random variables Y, Z we can bound the probability

$$\mathbb{P}_\theta(\theta \notin C_n, \mathcal{E}) = \mathbb{P}_\theta \left(\left\{ \frac{1}{2} \|\theta - \tilde{\theta}\|_F^2 > A + B + C + \frac{zd}{n} + \frac{\bar{z} + \xi_{\alpha/3, \sigma}}{\sqrt{n}} \right\}, \mathcal{E} \right)$$

by the sum of the following probabilities

$$I := \mathbb{P}_\theta \left(\left\{ \frac{1}{2} \|\theta - \tilde{\theta}\|_F^2 > \frac{1}{n} \|\mathcal{X}(\tilde{\theta} - \theta)\|^2 + \frac{zd}{n} \right\}, \mathcal{E} \right),$$

$$II := \mathbb{P}_\theta \left(\left\{ -\frac{1}{\sqrt{n}} \langle \varepsilon, \mathcal{X}(\theta - \tilde{\theta}) \rangle > \bar{z} \right\}, \mathcal{E} \right),$$

$$III := \mathbb{P}_\theta \left(-\frac{1}{\sqrt{n}} \sum_{i=1}^n (\varepsilon_i^2 - \mathbb{E}\varepsilon_i^2) > \xi_{\alpha/3, \sigma} \right).$$

The first probability I is bounded by

$$\begin{aligned} & \mathbb{P}_\theta \left(\left\{ -\frac{1}{n} \|\mathcal{X}(\tilde{\theta} - \theta)\|^2 + \|\theta - \tilde{\theta}\|_F^2 > \frac{1}{2} \|\theta - \tilde{\theta}\|_F^2 + \frac{zd}{n} \right\}, \mathcal{E} \right) \\ & \leq \mathbb{P}_\theta \left(\left\{ \left| \frac{1}{n} \|\mathcal{X}(\tilde{\theta} - \theta)\|^2 - \|\tilde{\theta} - \theta\|_F^2 \right| > \max \left(\frac{\|\theta - \tilde{\theta}\|_F^2}{2}, \frac{zd}{n} \right) \right\}, \mathcal{E} \right) = 0 \end{aligned}$$

About term II : Conditional on \mathcal{X} the variable $\frac{1}{\sqrt{n}} \langle \varepsilon, \mathcal{X}(\theta - \tilde{\theta}) \rangle$ is centred Gaussian with variance $(\sigma^2/n) \|\mathcal{X}(\theta - \tilde{\theta})\|^2$. The standard Gaussian tail bound then

gives by definition of \bar{z} , and conditional on \mathcal{X} ,

$$\begin{aligned} &\leq \exp\{-\bar{z}^2/2(\sigma^2/n)\|\mathcal{X}(\theta - \tilde{\theta})\|^2\} \\ &= \exp\left\{-\frac{z_{\alpha/3} \max(3\|\theta - \tilde{\theta}\|_F^2, 4zd/n)}{2\|\mathcal{X}(\theta - \tilde{\theta})\|^2/n}\right\} \leq \exp\{-z_{\alpha/3}\} = \alpha/3 \end{aligned}$$

since, on the event \mathcal{E} ,

$$\max(3\|\theta - \tilde{\theta}\|_F^2, 4zd/n) \geq (2/n)\|\mathcal{X}(\theta - \tilde{\theta})\|^2.$$

The overall bound for *II* follows from integrating the last but one inequality over the distribution of X . Term *III* is bounded by $\alpha/3$ by definition of $\xi_{\alpha,\sigma}$.

Remark 2 (Modification of the proof for Bernoulli errors) If instead of Gaussian errors we work with the error model from Subsection 2.3, we require a modified treatment of the terms *II*, *III* in the above proof. For the pure noise term *III* we modify the quantile constants slightly to $\xi_{\alpha,\sigma} = \sqrt{(1/\alpha)}$. If the number T of preparations satisfies $T \geq 4d^2$ then Chebyshev's inequality and (8) give

$$\mathbb{P}_\theta \left(\left| \frac{1}{\sqrt{n}} \sum_{i=1}^n (\varepsilon_i^2 - \mathbb{E}\varepsilon_i^2) \right| > \xi_{\alpha/3,\sigma} \right) \leq \frac{\alpha}{3n} \sum_{i=1}^n \mathbb{E}\varepsilon_i^4 \leq \frac{\alpha}{3} \frac{4d^2}{T} \leq \frac{\alpha}{3}.$$

For the 'cross term' we have likewise with $z_\alpha = \sqrt{1/\alpha}$ and $a_i = (\mathcal{X}(\theta - \tilde{\theta}))_i$ that, on the event \mathcal{E} ,

$$\begin{aligned} \mathbb{P}_\varepsilon \left(\left\{ -\frac{1}{\sqrt{n}} \langle \varepsilon, \mathcal{X}(\theta - \tilde{\theta}) \rangle > \bar{z} \right\}, \mathcal{E} \right) &\leq \frac{1}{n\bar{z}^2} \mathbb{E}_\varepsilon \left(\sum_{i=1}^n \varepsilon_i a_i 1_{\mathcal{E}} \right)^2 \\ &\leq \frac{d}{T\bar{z}^2} \frac{\|\mathcal{X}(\theta - \tilde{\theta})\|^2}{n} 1_{\mathcal{E}} \leq \alpha/3, \end{aligned}$$

just as at the end of the proof of Theorem 2, so that coverage follows from integrating the last inequality w.r.t. the distribution of X . The scaling $T \approx d^2$ is similar to the one discussed in Theorem 3 in ref. [10].

Lemma 1 *a) For isotropic design from Condition 1a) and any fixed matrix $\vartheta \in \mathbb{H}_d(\mathbb{C})$ we have, for every $n \in \mathbb{N}$,*

$$\Pr \left(\left| \frac{1}{n} \|\mathcal{X}\vartheta\|^2 - \|\vartheta\|_F^2 \right| > \frac{\|\vartheta\|_F^2}{2} \right) \leq 2e^{-cn}.$$

In the standard Gaussian design case we can take $c = 1/24$.

b) In the 'Pauli basis' case from Condition 1b) we have for any fixed matrix $\vartheta \in \mathbb{H}_d(\mathbb{C})$ satisfying the Schatten-1-norm bound $\|\vartheta\|_{S_1} \leq 2$ and every $n \in \mathbb{N}$,

$$\Pr \left(\left| \frac{1}{n} \|\mathcal{X}\vartheta\|^2 - \|\vartheta\|_F^2 \right| > \max \left(\frac{\|\vartheta\|_F^2}{2}, z \frac{d}{n} \right) \right) \leq 2 \exp \{-C(K)z\}$$

where $C(K) = 1/[(16 + 8/3)K^2]$, and where K is the coherence constant of the basis.

Proof. We first prove the isotropic case. From (4) we see

$$\Pr\left(\left|\frac{1}{n}\|\mathcal{X}\vartheta\|^2 - \|\vartheta\|_F^2\right| > \|\vartheta\|_F^2/2\right) = \Pr\left(\left|\sum_{i=1}^n (Z_i^2 - \mathbb{E}Z_1^2)/\|\vartheta\|_F^2\right| > n/2\right)$$

where the $Z_i/\|\vartheta\|_F$ are sub-Gaussian random variables. Then the $Z_i^2/\|\vartheta\|_F^2$ are sub-exponential and we can apply Bernstein's inequality (Prop. 4.1.8 in ref. [12]) to the last probability. We give the details for the Gaussian case and derive explicit constants. In this case $g_i := Z_i/\|\vartheta\|_F \sim N(0, 1)$ so the last probability is bounded, using Theorem 4.1.9 in ref. [12], by

$$\Pr\left(\left|\sum_{i=1}^n (g_i^2 - 1)\right| > \frac{n}{2}\right) \leq 2 \exp\left\{-\frac{n^2/4}{4n + 2n}\right\},$$

and the result follows.

Under Condition 1b), if we write $D = \max(n\|\vartheta\|_F^2/2, zd)$ we can reduce likewise to bound the probability in question by

$$\Pr\left(\left|\sum_{i=1}^n (Y_i - \mathbb{E}Y_1)\right| > D\right)$$

where the $Y_i = |\text{tr}(X^i\vartheta)|^2$ are i.i.d. bounded random variables. Using $\|E_i\|_{op} \leq K/\sqrt{d}$ from Condition 1b) and the quantum constraint $\|\vartheta\|_F \leq \|\vartheta\|_{S_1} \leq 2$ we can bound

$$|Y_i| \leq d^2 \max_i \|E_i\|_{op}^2 \|\vartheta\|_{S_1}^2 \leq 4K^2 d := U$$

as well as

$$\mathbb{E}Y_i^2 \leq U \mathbb{E}|Y_i| \leq 4K^2 d \|\vartheta\|_F^2 := s^2.$$

Bernstein's inequality for bounded variables (e.g., Theorem 4.1.7 in ref. [12]) applies to give the bound

$$2 \exp\left\{-\frac{D^2}{2ns^2 + \frac{2}{3}UD}\right\} \leq 2 \exp\{-C(K)z\},$$

after some basic computations, by distinguishing the two regimes of $D = n\|\vartheta\|_F^2/2 \geq zd$ and $D = zd \geq n\|\vartheta\|_F^2/2$. ■

5.3. Proof of Theorem 3

Since $\mathbb{E}_\theta \hat{R}_n = \|\theta - \tilde{\theta}\|_F^2$ we have from Chebyshev's inequality

$$\begin{aligned} \mathbb{P}_\theta(\theta \notin C_n) &\leq \mathbb{P}_\theta\left(|\hat{R}_n - \mathbb{E}\hat{R}_n| > z_{\alpha,n}\right) \\ &\leq \frac{\text{Var}_\theta(\hat{R}_n - \mathbb{E}\hat{R}_n)}{z_{\alpha,n}^2}. \end{aligned}$$

Now $U_n = \hat{R}_n - \mathbb{E}_\theta \hat{R}_n$ is a centred U-statistic and has Hoeffding decomposition $U_n = 2L_n + D_n$ where

$$L_n = \frac{1}{n} \sum_{i=1}^n \sum_{m,k} (Y_i X_{m,k}^i - \mathbb{E}_\theta [Y_i X_{m,k}^i]) (\Theta_{m,k} - \tilde{\Theta}_{m,k})$$

is the linear part and

$$D_n = \frac{2}{n(n-1)} \sum_{i < j} \sum_{m,k} (Y_i X_{m,k}^i - \mathbb{E}_\theta [Y_i X_{m,k}^i]) (Y_j X_{m,k}^j - \mathbb{E}_\theta [Y_j X_{m,k}^j])$$

the degenerate part. We note that L_n and D_n are orthogonal in $L^2(\mathbb{P}_\theta)$.

The linear part can be decomposed into $L_n = L_n^{(1)} + L_n^{(2)}$ where

$$L_n^{(1)} = \frac{1}{n} \sum_{i=1}^n \sum_{m,k} \left(\sum_{m',k'} X_{m',k'}^i X_{m,k}^i \Theta_{m',k'} - \Theta_{m,k} \right) (\Theta_{m,k} - \tilde{\Theta}_{m,k})$$

and

$$L_n^{(2)} = \frac{1}{n} \sum_{i=1}^n \varepsilon_i \sum_{m,k} X_{m,k}^i (\Theta_{m,k} - \tilde{\Theta}_{m,k}).$$

Now by the i.i.d. assumption we have

$$\text{Var}_\theta(L_n^{(2)}) = \sigma^2 \frac{\|\tilde{\theta} - \theta\|_F^2}{n}.$$

Moreover, by transposing the indices m, k and m', k' in an arbitrary way into single indices $M = 1, \dots, d^2, K = 1, \dots, d^2, d^2 = p$, respectively, basic computations given before eq. (28) in ref. [26] imply that the variance of the second term is bounded by

$$\text{Var}_\theta(L_n^{(1)}) \leq \frac{c \|\theta - \tilde{\theta}\|_F^2 \|\theta\|_F^2}{n}$$

where c is a constant that depends only on $\mathbb{E}X_{1,1}^4$ (which is finite since the $X_{1,1}$ are sub-Gaussian in view of Condition 1a)). Moreover, the degenerate term satisfies

$$\text{Var}_\theta(D_n) \leq c \frac{d}{n^2} \|\theta\|_F^4$$

in view of standard U-statistic computations leading to eq. (6.6) in ref. [19], with $d^2 = p$, and using the same transposition of indices as before. This proves coverage by choosing the constants in the definition of $z_{\alpha,n}$ large enough.

5.4. Proof of Theorem 4

We prove the result for symmetric matrices with real entries – the case of Hermitian matrices requires only minor (mostly notational) adaptations.

Given the estimator $\hat{\theta}_{\text{Pilot}}$, we can easily transform it into another estimator $\tilde{\theta}$ for which the following is true.

Theorem 5 *There exists an estimator $\tilde{\theta}$ that satisfies, uniformly in $\theta \in R(k)$, for any $k \leq d$ and with \mathbb{P}_θ -probability greater than $1 - 2\delta/3$,*

$$\|\tilde{\theta} - \theta\|_F \leq r_n(k),$$

as well as,

$$\tilde{\theta} \in R(k),$$

and then also

$$\|\tilde{\theta} - \theta\|_{S_1} \leq \sqrt{2k}r_n(k).$$

Proof. Let $\tilde{\theta}_{\text{Pilot}}$ and let $\tilde{\theta}$ be the element of $R(d)$ with smallest rank k' such that

$$\|\tilde{\theta}_{\text{Pilot}} - \tilde{\theta}\|_F^2 \leq \frac{r_n^2(k')}{4}.$$

Such $\tilde{\theta}$ exists and has rank $\leq k$, with probability $\geq 1 - 2\delta/3$, since $\theta \in R(k)$ satisfies the above inequality in view of (23). The $\|\cdot\|_F^2$ -loss of $\tilde{\theta}$ is no larger than $r_n(k)$ by the triangle inequality

$$\|\tilde{\theta} - \theta\|_F \leq \|\tilde{\theta} - \tilde{\theta}_{\text{Pilot}}\|_F + \|\tilde{\theta}_{\text{Pilot}} - \theta\|_F,$$

and this completes the proof of the third claim in view of (2). ■

The rest of the proof consists of three steps: The first establishes some auxiliary empirical process type results, which are then used in the second step to construct a sufficiently good simultaneous estimate of the eigenvalues of θ . In Step III the coverage of the confidence set is established.

STEP I

Let $\theta \in R^+(k) = R(k) \cap \Theta_+$ and let $\tilde{\theta}$ be the estimator from Theorem 5. Then with probability $\geq 1 - 2\delta/3$, and if $\eta = \tilde{\theta} - \theta$, we have

$$\|\eta\|_F^2 \leq r_n^2(k) \quad \forall \theta \in R^+(k), \tag{27}$$

and that $\eta \in R(2k)$. For the rest of the proof we restrict in what follows to the event of probability greater than or equal to $1 - 2\delta/3$ described by a) and b) in the hypothesis of the theorem.

Write $Y'_i = Y_i - \text{tr}(X^i \tilde{\theta})$ for the ‘new observations’

$$Y'_i = \text{tr}(X^i \eta) + \varepsilon_i, \quad i = 1, \dots, n.$$

For any $d \times d'$ matrix V we set

$$\tilde{\gamma}_\eta(V) = V^T \left(\frac{1}{n} \sum_{i=1}^n X^i Y'_i \right) V$$

which estimates

$$\gamma_\eta(V) = V^T \eta V.$$

Let now U be any unit vector in \mathbb{R}^d . Then in the above notation ($d' = 1$) we can write

$$\begin{aligned}\tilde{\gamma}_\eta(U) &= \frac{1}{n} \sum_{i=1}^n \sum_{m,m' \leq d} U_m U_{m'} X_{m,m'}^i Y_i' \\ &= \frac{1}{n} \sum_{i=1}^n \sum_{m,m' \leq d} U_m U_{m'} X_{m,m'}^i (\text{tr}(X^i \eta) + \varepsilon_i) \\ &= \frac{1}{n} \sum_{i=1}^n \sum_{m,m' \leq d} U_m U_{m'} X_{m,m'}^i \left(\sum_{k,k' \leq d} X_{k,k'}^i \eta_{k,k'} + \varepsilon_i \right).\end{aligned}$$

If \mathbb{U} denotes the $d \times d$ matrix UU^T , the last quantity can be written as

$$\frac{1}{n} \langle \mathcal{X} \mathbb{U}, \mathcal{X} \eta \rangle + \frac{1}{n} \langle \mathcal{X} \mathbb{U}, \varepsilon \rangle.$$

We can hence bound, for $\mathcal{S} = \{U \in \mathbb{R}^d : \|U\|_2 = 1\}$

$$\begin{aligned}& \sup_{\eta \in R(2k), \|\eta\|_F \leq r_n(k), U \in \mathcal{S}} |\tilde{\gamma}_\eta(U) - \gamma_\eta(U)| \\ & \leq \sup_{\eta \in R(2k), \|\eta\|_F \leq r_n(k), U \in \mathcal{S}} \left| \frac{1}{n} \langle \mathcal{X} \mathbb{U}, \mathcal{X} \eta \rangle - \langle \mathbb{U}, \eta \rangle \right| + \sup_{U \in \mathcal{S}} \left| \frac{1}{n} \langle \mathcal{X} \mathbb{U}, \varepsilon \rangle \right|.\end{aligned}$$

Lemma 2 *The right hand side on the last inequality is, with probability greater than $1 - \delta$, of order*

$$v_n := O \left(r_n(k) \tau_n(k) + \sqrt{\frac{d}{n}} \right).$$

Proof. The first term in the bound corresponds to the first supremum on the right hand side of the last inequality, and follows directly from the matrix RIP (and Lemma 4). For the second term we argue conditionally on the values of \mathcal{X} and on the event for which the matrix RIP is satisfied. We bound the supremum of the Gaussian process

$$\mathbb{G}_\varepsilon(U) := \frac{1}{\sqrt{n}} \langle \mathcal{X} \mathbb{U}, \varepsilon \rangle \sim N(0, \|\mathcal{X} \mathbb{U}\|^2/n)$$

indexed by elements U of the unit sphere \mathcal{S} of \mathbb{R}^d , which satisfies the metric entropy bound

$$\log N(\delta, \mathcal{S}, \|\cdot\|) \lesssim d \log(A/\delta)$$

by a standard covering argument. Moreover $\mathbb{U} = UU^T \in R(1)$ and hence for any pair of vectors $U, \bar{U} \in \mathcal{S}$ we have that $\mathbb{U} - \bar{\mathbb{U}} \in R(2)$. From the RIP we deduce for every fixed $U, \bar{U} \in \mathcal{S}$ that

$$\begin{aligned}\frac{1}{n} \|\mathcal{X} \mathbb{U} - \mathcal{X} \bar{\mathbb{U}}\|^2 &= \|\mathbb{U} - \bar{\mathbb{U}}\|_F^2 \left(1 + \frac{\frac{1}{n} \|\mathcal{X}(\mathbb{U} - \bar{\mathbb{U}})\|^2 - \|\mathbb{U} - \bar{\mathbb{U}}\|_F^2}{\|\mathbb{U} - \bar{\mathbb{U}}\|_F^2} \right) \\ &\leq (1 + \tau_n(2)) \|\mathbb{U} - \bar{\mathbb{U}}\|_F^2 \leq C \|U - \bar{U}\|^2\end{aligned}$$

since $\tau_n(2) = O(1)$ and since

$$\begin{aligned} \|U - \bar{U}\|_F^2 &= \sum_{m,m'} (U_m U_{m'} - \bar{U}_m \bar{U}_{m'})^2 \\ &= \sum_{m,m'} (U_m U_{m'} - U_m \bar{U}_{m'} + U_m \bar{U}_{m'} - \bar{U}_m \bar{U}_{m'})^2 \leq 2\|U - \bar{U}\|^2. \end{aligned}$$

Hence any δ -covering of \mathcal{S} in $\|\cdot\|$ induces a δ/C covering of \mathcal{S} in the intrinsic covariance $d_{\mathbb{G}_\varepsilon}$ of the (conditional on \mathcal{X}) Gaussian process \mathbb{G}_ε , i.e.,

$$\log N(\delta, \mathcal{S}, d_{\mathbb{G}_\varepsilon}) \lesssim d \log(A'/\delta)$$

with constants independent of X . By Dudley's metric entropy bound (e.g., ref. [12]) applied to the conditional Gaussian process we have for $D > 0$ some constant

$$\mathbb{E} \sup_{U \in \mathcal{S}} |\mathbb{G}_\varepsilon(U)| \lesssim \int_0^D \sqrt{\log N(\delta, \mathcal{S}, d_{\mathbb{G}_\varepsilon})} d\delta \lesssim \sqrt{d}$$

and hence we deduce that

$$\mathbb{E}_\varepsilon \sup_{U \in \mathcal{S}} \frac{1}{n} |\langle \mathcal{X}U, \varepsilon \rangle| = \mathbb{E}_\varepsilon \frac{1}{\sqrt{n}} \sup_{U \in \mathcal{S}} |\mathbb{G}_\varepsilon(U)| \lesssim \sqrt{\frac{d}{n}} \quad (28)$$

with constants independent of X , so that the result follows from applying Markov's inequality. ■

STEP II:

Define the estimator

$$\hat{\theta}' = \tilde{\theta} + \frac{1}{n} \sum_{i=1}^n X^i Y_i' = \tilde{\theta} + \tilde{\gamma}_\eta(I_d).$$

Then we can write, using $U^T \tilde{\gamma}_\eta(I_d)U = \tilde{\gamma}_\eta(U)$,

$$\begin{aligned} U^T \hat{\theta}'U - U^T \theta U &= U^T (\tilde{\theta} + \tilde{\gamma}_\eta(I_d))U - U^T (\tilde{\theta} + \eta)U \\ &= \tilde{\gamma}_\eta(U) - \gamma_\eta(U), \end{aligned}$$

and from the previous lemma we conclude, for any unit vector U that with probability $\geq 1 - \delta$,

$$|U^T \hat{\theta}'U - U^T \theta U| \leq v_n.$$

Let now $\hat{\theta}$ be any symmetric positive definite matrix such that

$$|U^T \hat{\theta}U - U^T \hat{\theta}'U| \leq v_n.$$

Such a matrix exists, for instance $\theta \in R^+(k)$, and by the triangle inequality we also have

$$|U^T \hat{\theta}U - U^T \theta U| \leq 2v_n. \quad (29)$$

Lemma 3 *Let M be a symmetric positive definite $d \times d$ matrix with eigenvalues λ_j 's ordered such that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$. For any $j \leq d$ consider an arbitrary collection of j orthonormal vectors $\mathcal{V}_j = (V^\iota : 1 \leq \iota \leq j)$ in \mathbb{R}^d . Then we have*

$$a) \quad \lambda_{j+1} \leq \sup_{U \in \mathcal{S}, U \perp \text{span}(\mathcal{V}_j)} U^T M U,$$

and

$$b) \quad \sum_{\iota \leq j} \lambda_\iota \geq \sum_{\iota \leq j} (V^\iota)^T M V^\iota.$$

The proof of this lemma is basic and given in the appendix. Let now \hat{R} be the rotation that diagonalises $\hat{\theta}$ such that $\hat{R}^T \hat{\theta} \hat{R} = \text{diag}(\hat{\lambda}_j : j = 1, \dots, d)$ ordered such that $\hat{\lambda}_j \geq \hat{\lambda}_{j+1} \forall j$. Moreover let R be the rotation that does the same for θ and its eigenvalues λ_j . We apply the previous lemma with $M = \hat{\theta}$ and \mathcal{V} equal to the column vectors $r_\iota : \iota \leq l-1$ of R to obtain, for any fixed $l \leq j \leq d$,

$$\hat{\lambda}_l \leq \sup_{U \in \mathcal{S}, U \perp \text{span}(r_\iota, \iota \leq l-1)} U^T \hat{\theta} U, \quad (30)$$

and also that

$$\sum_{l \leq j} \hat{\lambda}_l \geq \sum_{l \leq j} r_l^T \hat{\theta} r_l. \quad (31)$$

From (29) we deduce, that

$$\hat{\lambda}_l \leq \sup_{U \in \mathcal{S}, U \perp \text{span}(r_\iota, \iota \leq j-1)} U^T \theta U + 2v_n = \lambda_j + 2v_n \quad \forall l \leq j,$$

as well as

$$\sum_{l \leq j} \hat{\lambda}_l \geq \sum_{l \leq j} r_l^T \theta r_l - 2jv_n = \sum_{l \leq j} \lambda_l - 2jv_n,$$

with probability $\geq 1 - \delta$. Combining these bounds we obtain

$$\left| \sum_{l \leq j} \hat{\lambda}_l - \sum_{l \leq j} \lambda_l \right| \leq 2jv_n, \quad j \leq d. \quad (32)$$

STEP III

We show that the confidence sets covers the true parameter on the event of probability $\geq 1 - \delta$ on which Steps I and II are valid, and for the constant C chosen large enough.

Let $\Pi = \Pi_{R^+(2\hat{k})}$ be the projection operator onto $R^+(2\hat{k})$. We have

$$\|\hat{\vartheta} - \theta\|_{S_1} \leq \|\hat{\vartheta} - \Pi\theta\|_{S_1} + \|\Pi\theta - \theta\|_{S_1}.$$

We have, using (32) and Lemma 5 below

$$\begin{aligned} \|\Pi\theta - \theta\|_{S_1} &= \sum_{J>2\hat{k}} \lambda_J = 1 - \sum_{J\leq 2\hat{k}} \lambda_J \\ &\leq 1 - \sum_{J\leq 2\hat{k}} \hat{\lambda}_J + 4\hat{k}v_n \\ &\leq 6v_n\hat{k} \leq (C/2)\sqrt{\hat{k}r_n(\hat{k})} \end{aligned}$$

for C large enough.

Moreover, using the oracle inequality (24) with $S = \Pi\theta$ and (25),

$$\begin{aligned} \|\hat{\vartheta} - \Pi\theta\|_{S_1} &\leq \sqrt{4\hat{k}}\|\hat{\vartheta} - \Pi\theta\|_F \\ &\leq \sqrt{4\hat{k}}(\|\hat{\vartheta} - \theta\|_F + \|\Pi\theta - \theta\|_F) \\ &\leq \sqrt{4\hat{k}}(\|\hat{\vartheta} - \tilde{\theta}_{\text{Pilot}}\|_F + \|\tilde{\theta}_{\text{Pilot}} - \theta\|_F + \|\Pi\theta - \theta\|_F) \\ &\lesssim \sqrt{\hat{k}}(r_n(\hat{k}) + \|\Pi\theta - \theta\|_F). \end{aligned}$$

We finally deal with the approximation error: Note

$$\|\Pi\theta - \theta\|_F^2 = \sum_{l>2\hat{k}} \lambda_l^2 \leq \max_{l>2\hat{k}} |\lambda_l| \sum_{l>2\hat{k}} |\lambda_l|.$$

By (32) we know that

$$\sum_{l>\hat{k}} \lambda_l = 1 - \sum_{l\leq\hat{k}} \lambda_l \leq 1 - \sum_{l\leq\hat{k}} \hat{\lambda}_l + 2v_n\hat{k} \leq 4v_n\hat{k}.$$

Hence out of the λ_l 's with indices $l > \hat{k}$ there have to be less than \hat{k} coefficients which exceed $4v_n$. Since the eigenvalues are ordered this implies that the λ_l 's with indices $l > 2\hat{k}$ are all less than or equal to $4v_n$, and hence the quantity in the last but one display is bounded by (since $\hat{k} < 2\hat{k}$), using again (32) and the definition of \hat{k} ,

$$4v_n \left(1 - \sum_{l\leq\hat{k}} |\lambda_l| \right) \lesssim v_n \left(1 - \sum_{l\leq\hat{k}} |\hat{\lambda}_l| \right) + \hat{k}v_n^2 \lesssim v_n^2\hat{k} \lesssim \sqrt{\hat{k}r_n(\hat{k})}.$$

Overall we get the bound

$$\|\hat{\vartheta} - \Pi\theta\|_{S_1} \lesssim \hat{k}v_n \lesssim (C/2)\sqrt{\hat{k}r_n(\hat{k})}$$

for C large enough, which completes the proof of coverage of C_n by collecting the above bounds. The diameter bound follows from $\hat{k} \leq k$ (in view of the defining inequalities of \hat{k} being satisfied, for instance, for $\tilde{\theta}' = \theta$, whenever $\theta \in R^+(k_0)$.)

We conclude with the following auxiliary results used above.

Lemma 4 Under the RIP (6) we have for every $1 \leq k \leq d$ that, with probability at least $1 - \delta$,

$$\sup_{A, B \in R(k)} \left| \frac{\frac{1}{n} \langle \mathcal{X}A, \mathcal{X}B \rangle - \langle A, B \rangle_F}{\|A\|_F \|B\|_F} \right| \leq 10\tau_n(k). \quad (33)$$

Proof. The matrix RIP can be written as

$$\sup_{A \in R(k)} \left| \frac{\langle \mathcal{X}A, \mathcal{X}A \rangle}{n \langle A, A \rangle_F} - 1 \right| = \frac{|\langle A, (n^{-1}M - \mathbb{I})A \rangle_F|}{\langle A, A \rangle_F} \leq \tau_n(k), \quad (34)$$

for a suitable $M \in \mathbb{H}_{d^2}(\mathbb{C})$. The above bound then follows from applying the Cauchy-Schwarz inequality to

$$\frac{1}{n} \langle \mathcal{X}A, \mathcal{X}B \rangle - \langle A, B \rangle_F = \langle A, (n^{-1}M - \mathbb{I})B \rangle_F. \quad (35)$$

■

The proof of the following basic lemma is left to the reader.

Lemma 5 Let $M \geq 0$ with positive eigenvalues $(\lambda_j)_j$ ordered in decreasing order. Denote with $\Pi_{R^+(j-1)}$ the projection onto $R^+(j-1) = R(j-1) \cap \Theta_+$. Then for any $2 \leq j \leq d$ we have

$$\sum_{j' \geq j} \lambda_{j'} = \|M - \Pi_{R^+(j-1)}M\|_{S_1}.$$

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6. Appendix

6.1. Pauli spin measurements & Quantum Tomography

This work was partly motivated by a problem arising in present-day physics experiments that aim at estimating quantum states. Conceptually, a quantum mechanical experiment involves two stages: A *source* (or *preparation procedure*) that emits quantum mechanical systems with unknown properties, and a *measurement device* that interacts with incoming quantum systems and produces real-valued measurement outcomes, e.g. by pointing a dial to a value on a scale. Quantum mechanics stipulates that both stages are completely described by certain matrices.

The properties of the source are represented by a positive semi-definite unit trace matrix θ , the *quantum state*, also referred to as *density matrix*. In turn, the measurement device is modelled by a Hermitian matrix X , which is referred to as an *observable* in physics jargon. A key axiom of the quantum mechanical formalism states that if the measurement X is repeatedly performed on systems emitted by the source that is preparing θ , then the real-valued measurement outcomes will fluctuate randomly with expected value

$$\langle X, \theta \rangle_F = \text{tr}(X\theta). \tag{36}$$

The precise way in which physical properties are represented by these matrices is immaterial to our discussion (cf. any textbook, e.g. ref. [28]). We merely note

that, while in principle *any* Hermitian X can be measured by some physical apparatus, the required experimental procedures are prohibitively complicated for all but a few highly structured matrices. This motivates the introduction of *Pauli designs* below, which correspond to fairly tractable ‘spin measurements’.

The *quantum state estimation* or *quantum tomography*¹ problem is to estimate an unknown density matrix θ from the measurement of a collection of observables X^1, \dots, X^n . This task is of particular importance to the young field of quantum information science [27]. There, the sources might be carefully engineered components used for technological applications such as quantum key distribution or quantum computing. In this context, quantum state estimation is the process of characterising the components one has built – clearly an important capability for any technology.

A major challenge lies in the fact that relevant instances are described by $d \times d$ -matrices for fairly large dimensions d ranging from 100 to 10.000 in presently performed experiments [16]. Such high-dimensional estimation problems can benefit substantially from structural properties of the objects to be recovered. Fortunately, the density matrices occurring in quantum information experiments are typically well-approximated by matrices of *low rank* $r \ll d$. In fact, in the practically most important applications, one usually even aims at preparing a state of unit rank – a so-called *pure quantum state*.

6.1.1. Pauli observables

We now introduce a paradigmatic set of quantum measurements that is frequently used in both theoretical and practical treatments of quantum state estimation (see, e.g., refs. [14, 16]). For a more general account, we refer to standard textbooks [18, 27]. The purpose of this section is to motivate the ‘Pauli design’ case (Condition 1b) of the main theorem, as well as the approximate Gaussian noise model described in Subsection 2.3.

We start by describing ‘spin measurements’ on a single ‘spin-1/2 particle’. Such a measurement corresponds to the situation of having $d = 2$. Without worrying about the physical significance, we accept as fact that on such particles, one may measure one of three properties, referred to as the ‘spin along the x, y , or z -axis’ of \mathbb{R}^3 . Each of these measurements may yield one of two outcomes, denoted by $+1$ and -1 respectively.

The mathematical description of these measurements is derived from the *Pauli matrices*

$$\sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (37)$$

¹ The term ‘tomography’ goes back to the use of *Radon transforms* in early schemes for estimating quantum states of electromagnetic fields [23, 1]. It has become synonymous with ‘quantum density matrix estimation’, even though current methods applied to quantum systems with a finite dimension d have no technical connection to classical tomographic reconstruction algorithms.

in the following way. Recall that the Pauli matrices have eigenvalues ± 1 . For $x \in \{1, 2, 3\}$ and $j \in \{+1, -1\}$, we write ψ_j^x for the normalised eigenvector of σ^x with eigenvalue j . The spectral decomposition of each Pauli spin matrix can hence be expressed as

$$\sigma^x = \pi_+^x - \pi_-^x, \quad (38)$$

with

$$\pi_\pm^x = \psi_\pm^x (\psi_\pm^x)^* \geq 0 \quad (39)$$

denoting the projectors onto the eigenspaces. Now, a physical measurement of the ‘spin along direction x ’ on a system in state θ will give rise to a $\{-1, 1\}$ -valued random variable C^x with

$$\mathbb{P}(C^x = j) = \text{tr}(\pi_j^x \theta), \quad (40)$$

where $\theta \in \mathbb{H}_2(\mathbb{C})$. Using eq. (38), this is equivalent to stating that the expected value of C^x is given by

$$\mathbb{E}(C^x) = \text{tr}(\sigma^x \theta). \quad (41)$$

Next, we consider the case of joint spin measurements on a collection of N particles. For each, one has to decide on an axis for the spin measurement. Thus, the joint *measurement setting* is now described by a word $x = (x_1, \dots, x_N) \in \{1, 2, 3\}^N$. The axioms of quantum mechanics posit that the joint state θ of the N particles acts on the tensor product space $(\mathbb{C}^2)^{\otimes N}$, so that $\theta \in \mathbb{H}_{2^N}(\mathbb{C})$.

Likewise, the *measurement outcome* is a word $j = (j_1, \dots, j_N) \in \{1, -1\}^N$, with j_i the value of the spin along axis x_i of particle $i = 1, \dots, N$. As above, this prescription gives rise to a $\{1, -1\}^N$ -valued random variable C^x . Again, the axioms of quantum mechanics imply that the distribution of C^x is given by

$$\mathbb{P}(C^x = j) = \text{tr}((\pi_{j_1}^{x_1} \otimes \dots \otimes \pi_{j_N}^{x_N})\theta). \quad (42)$$

Note that the components of the random vector C^x are not necessarily independent, as θ will generally not factorise

It is often convenient to express the information in eq. (42) in a way that involves tensor products of Pauli matrices, rather than their spectral projections. In other words, we seek a generalisation of eq. (41) to N particles. As a first step toward this goal, let

$$\chi(j) = \begin{cases} -1 & \text{number of } -1 \text{ elements in } j \text{ is odd} \\ 1 & \text{number of } -1 \text{ elements in } j \text{ is even} \end{cases} \quad (43)$$

be the *parity function*. Then one easily verifies

$$\text{tr}((\sigma^{x_1} \otimes \dots \otimes \sigma^{x_N})\theta) = \sum_{j \in \{1, -1\}^N} \chi(j) \text{tr}(\theta(\pi_{j_1}^{x_1} \otimes \dots \otimes \pi_{j_N}^{x_N})) = \mathbb{E}(\chi(C^x)). \quad (44)$$

In this sense, the tensor product $\sigma^{x_1} \otimes \dots \otimes \sigma^{x_N}$ describes a measurement of the parity of the spins along the respective directions given by x .

In fact, the entire distribution of C^x can be expressed in terms of tensor products of Pauli matrices and suitable parity functions. To this end, we extend the definitions above. Write

$$\sigma^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (45)$$

for the identity matrix in $\mathbb{M}_2(\mathbb{C})$. For every subset S of $\{1, \dots, N\}$, define the ‘parity function restricted to S ’ via

$$\chi_S(j) = \begin{cases} -1 & \text{number of } -1 \text{ elements } j_i \text{ for } i \in S \text{ is odd} \\ 1 & \text{number of } -1 \text{ elements } j_i \text{ for } i \in S \text{ is even.} \end{cases} \quad (46)$$

Lastly, for $S \subset \{1, \dots, N\}$ and $x \in \{1, 2, 3\}^N$, the *restriction of x to S* is

$$x_i^S = \begin{cases} x_i & i \in S \\ 0 & i \notin S. \end{cases} \quad (47)$$

Then for every such x, S one verifies the identity

$$\text{tr}((\sigma^{x_1^S} \otimes \dots \otimes \sigma^{x_N^S})\theta) = \mathbb{E}(\chi_S(C^x)). \quad (48)$$

In other words, the distribution of C^x contains enough information to compute the expectation value of all observables $(\sigma^{x_1^S} \otimes \dots \otimes \sigma^{x_N^S})$ that can be obtained by replacing the Pauli matrices on an arbitrary subset S of particles by the identity σ^0 . The converse is also true: the set of all such expectation values allows one to recover the distribution of C^x . The explicit formula reads

$$\begin{aligned} \mathbb{P}(C^x = j) &= \frac{1}{2^N} \sum_{S \subset \{1, \dots, N\}} \chi_S(j) \mathbb{E}(\chi_S(C^x)) \\ &= \frac{1}{2^N} \sum_{S \subset \{1, \dots, N\}} \chi_S(j) \text{tr}(\theta(\sigma^{x_1^S} \otimes \dots \otimes \sigma^{x_N^S})) \end{aligned} \quad (49)$$

and can be verified by direct computation. [Note that $\mathbb{E}(\chi_S(C^x))$ is effectively a Fourier coefficient (over the group \mathbb{Z}_2^N) of the distribution function of the $\{-1, 1\}^N$ -valued random variable C^x . Equation (49) is then nothing but an inverse Fourier transform.]

In this sense, the information obtainable from joint spin measurements on N particles can be encoded in the 4^N real numbers

$$2^{-N/2} \text{tr}((\sigma^{y_1} \otimes \dots \otimes \sigma^{y_N})\theta), \quad y \in \{0, 1, 2, 3\}^N. \quad (50)$$

Indeed, every such y arises as $y = x^S$ for some (generally non-unique) combination of x and S . This representation is particularly convenient from a mathematical point of view, as the collection of matrices

$$E^y := 2^{-N/2} \sigma^{y_1} \otimes \dots \otimes \sigma^{y_N}, \quad y \in \{0, 1, 2, 3\}^N \quad (51)$$

forms an ortho-normal basis with respect to the $\langle \cdot, \cdot \rangle_F$ inner product. Thus the terms in eq. (50) are just the coefficients of a basis expansion of the density matrix θ .²

6.1.2. From (50) to Condition 1b)

Following [10] we use eq. (50) as our model for quantum tomographic measurements. Note that the E^y satisfy Condition 1b) with coherence constant $K = 1$ and $d = 2^N$. In the model (1) under Condition 1b) we wish to approximate $d \cdot \text{tr}(E^y \theta)$ for a fixed observable E^y (we fix the random values of the X^i 's here) and for $d = 2^N$. If $y = x^S$ for some setting x and subset S , then the parity function $B^y := \chi_S(C^x)$ has expected value $2^{N/2} \cdot \text{tr}(E^y \theta) = \sqrt{d} \cdot \text{tr}(E^y \theta)$ (see eqs. (48) and (51)), and itself is a Bernoulli variable taking values $\{1, -1\}$ with

$$p = \mathbb{P}(B^y = 1) = \frac{1 + \sqrt{d} \text{tr}(E^y \theta)}{2}.$$

Note that

$$\sqrt{d} |\text{tr}(E^y \theta)| \leq \sqrt{d} \|E^y\|_{op} \|\theta\|_{S_1} \leq 1,$$

so indeed $p \in [0, 1]$ and the variance satisfies

$$\text{Var} B^y = 1 - d \cdot \text{tr}(E^y \theta)^2 \leq 1.$$

This is precisely the error model described in Subsection 2.3.

6.2. Proof of Lemma 3

a): Consider the subspaces $E = \text{span}((V^t)_{t \leq j})^\perp$ and $F = \text{span}((e_t)_{t \leq j+1})$ of \mathbb{R}^d , where the e_t 's are the eigenvectors of the $d \times d$ matrix M corresponding to eigenvalues λ_j . Since $\dim(E) + \dim(F) = (d - j) + j + 1 = d + 1$, we know that $E \cap F$ is not empty and there is a vectorial sub-space of dimension 1 in the intersection. Take $U \in E \cap F$ such that $\|U\| = 1$. Since $U \in F$, it can be written as

$$U = \sum_{t=1}^{j+1} u_t e_t$$

for some coefficients u_t . Since the e_t 's are orthogonal eigenvectors of the symmetric matrix M we necessarily have

$$MU = \sum_{t=1}^{j+1} \lambda_t u_t e_t,$$

²We note that quantum mechanics allows to design measurement devices that directly probe the observable of $\sigma^{y_1} \otimes \dots \otimes \sigma^{y_N}$, without first measuring the spin of every particle and then computing a parity function. In fact, the ability to perform such correlation measurements is crucial for *quantum error correction protocols* [27]. For practical reasons these setups are used less commonly in tomography experiments, though.

and thus

$$U^T M U = \sum_{\iota=1}^{j+1} \lambda_{\iota} u_{\iota}^2.$$

Since the λ_{ι} 's are all non-negative and ordered in decreasing absolute value, one has

$$U^T M U = \sum_{\iota=1}^{j+1} \lambda_{\iota} u_{\iota}^2 \geq \lambda_{j+1} \sum_{\iota=1}^{j+1} u_{\iota}^2 = \lambda_{j+1} \|U\|^2 = \lambda_{j+1}.$$

Taking the supremum in U yields the result.

b): For each $\iota \leq j$, let us write the decomposition of V^{ι} on the basis of eigenvectors ($e_l : l \leq d$) of M as

$$V^{\iota} = \sum_{l \leq d} v_l^{\iota} e_l.$$

Since the (e_l) are the eigenvectors of M we have

$$\sum_{\iota \leq j} (V^{\iota})^T M V^{\iota} = \sum_{\iota \leq j} \sum_{l=1}^d \lambda_l (v_l^{\iota})^2,$$

where $\sum_{l=1}^d (v_l^{\iota})^2 = 1$ and $\sum_{\iota \leq j} (v_l^{\iota})^2 \leq 1$, since the V^{ι} are orthonormal. The last expression is maximised in $(v_l^{\iota})_{\iota \leq j, 1 \leq l \leq d}$ and under these constraints, when $v_l^{\iota} = 1$ and $v_l^{\iota} = 0$ if $\iota \neq l$ (since the (λ_l) are in decreasing order), and this gives

$$\sum_{\iota \leq j} (V^{\iota})^T M V^{\iota} \leq \sum_{\iota \leq j} \lambda_{\iota}.$$