Quantum algorithms for spectral sums

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Abstract

We propose and analyze new quantum algorithms for estimating the most common spectral sums of symmetric positive definite (SPD) matrices. For a function $f$ and a matrix $A \in \mathbb{R}^{n \times n}$, the spectral sum is defined as $S_f(A) := \text{Tr}[f(A)] = \sum_j f(\lambda_j)$, where $\lambda_j$ are the eigenvalues. Examples of spectral sums are the von Neumann entropy, the trace of inverse, the log-determinant, and the Schatten-$p$ norm, where the latter does not require the matrix to be SPD. The fastest classical randomized algorithms estimate these quantities have a runtime that depends at least linearly on the number of nonzero components of the matrix. Assuming quantum access to the matrix, our algorithms are sub-linear in the matrix size, and depend at most quadratically on other quantities, like the condition number and the approximation error, and thus can compete with most of the randomized and distributed classical algorithms proposed in recent literature. These algorithms can be used as subroutines for solving many practical problems, for which the estimation of a spectral sum often represents a computational bottleneck.

1 Introduction

The trace of matrix function, far from being only of theoretical interest, appears in many practical applications of linear algebra. To name a few, it has applications in machine learning, computational chemistry, biology, statistics, finance, and many others [1, 6, 13, 14, 24, 26, 31, 49, 52, 53]. While the problem of estimating some spectral quantities dates back to decades, many fast classical algorithms have been developed recently [7, 28, 29, 38, 47, 58, 61], highlighting the importance of spectral sums in many numerical problems.

The spectral sum is defined as the sum of the eigenvalues of a matrix after a given function is applied to them. Oftentimes, the matrix will be symmetric positive definite (SPD), but there are cases where this assumption is relaxed. As an example, the logarithm of the determinant is perhaps the most common example of spectral sum, as the determinant is one of the most important properties associated with a matrix. However, the standard definition does not offer an efficient way of computing it. Remarkably, it is often the case that the logarithm of the determinant is the quantity that is effectively needed in the applications, which is much more amenable to estimation.

Definition 1 (Spectral sum [28, 59]). Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix with $A = U DU^\dagger$ its eigenvalues decomposition, where $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$ is the diagonal matrix of the eigenvalues, and $f : \mathbb{R} \mapsto \mathbb{R}$ is a function. The spectral sum of $A$ for the function $f$ is defined as:

$$S_f(A) := \text{Tr}[f(A)] = \sum_{j=1}^n f(\lambda_j).$$ 

(1)
In case the matrix is not SPD, the spectral sum of a matrix can be defined on the singular values. This is the case for Schatten-$p$ norms, discussed in section 2.3.

In the last decades, quantum information emerged as a new paradigm of computation, which is expected to offer faster-than-classical algorithms. In 2009 the HHL algorithm [32] represented a breakthrough in quantum information processing, as it was the first quantum algorithm that proposed a way to solve a linear system of equations in a runtime that is only poly-logarithmic in the size of the system (and polynomial in other parameters, like the sparsity and the condition number). After a decade, these techniques have been considerably improved, [11, 23, 40], and a whole ecosystem of algorithms for quantum linear algebra have emerged, further improving upon the runtime dependence on parameters like the error, and the condition number. The value of quantum algorithms lies in the asymptotic scaling of their runtime, which should depend only polylogarithmically on the size of the dataset, and polynomially on other parameters.

In this work we study new quantum algorithms for computing the spectral sums like the log-determinant, the von Neumann entropy, the trace of the inverse, and the Schatten-$p$ norm of a matrix. The manuscript is organized as follows. In this section, we report some previous classical and quantum works, and we introduce the notation and preliminaries, and we discuss briefly our results. In section 2 we present the main theorems and the algorithms for the spectral sums. The appendix is organized as follows. First we introduce more preliminaries used in the proofs and in the algorithms, like the trace estimation subroutines. We proceed by discussing some other quantum algorithms for the log-determinant based on different techniques and we discuss their comparison and improvements upon previous works.

1.1 Previous works

In the past three decades, several classical algorithms for spectral sums have been proposed, e.g. [28, 47, 58]. We list here the various approaches that have been explored in the literature, while we will call up the runtimes of the best classical algorithm for a spectral sum in each of the appropriate sections. The vast majority of the classical algorithms for spectral sums rely on a stochastic algorithm for trace estimation [3], and a technique of polynomial approximation.

The log-determinant of a matrix is highly studied in classical literature. The first result was based on the Taylor expansions and the stochastic trace estimator [5], while others featured some error compensation schemes for improving the accuracy [64]. A few years later, Pace et al. built upon the results of [44], and used the Chebyshev approximation of the logarithm function, albeit with exact trace calculation algorithm [51], and without proposing a convergence analysis of the algorithm. Similar to Pace et al., in 2015, Boutsidis et al. [7] improved previous results using the Taylor expansion of the logarithm function and used the power method to estimate the biggest singular value of a matrix. They also used stochastic trace approximation instead of exact trace computation algorithms. In 2014, Aune et al. kept relying on trace estimation techniques, but integrated results from complex analysis, namely the Cauchy integral, for approximating the logarithm function [2]. In [29], they were the first to combine trace estimators and Chebyshev approximation algorithms. For von Neumann entropy - similar in spirit to the algorithms mentioned for the log-determinant - three randomized algorithms are given in [38]. They use stochastic trace estimation, Taylor approximation and Chebyshev approximation. For results on the trace of the inverse we refer to [61].

There are already some quantum algorithms that have been used to estimate some of the spectral sums. For instance, there is a vast literature on quantum algorithms for estimating von Neumann entropies in various models, (and more generally Rényi entropies [22, 39, 56]). In quantum information, the trace of a matrix has been approximated in many different contexts [9, 56]. The work of [9], which has been used to estimate the Schatten-$p$ norm, is not directly comparable to the results presented here, as they use a restricted model of quantum computation. The algorithm most similar to our work is due to Zhao et al., [65, 66], where the authors develop a sampling-based algorithm to estimate the log-determinant and the Schatten-$p$ norms of matrices. We reanalyze the runtime of their algorithm, study the variance of their estimator, and improve it using faster quantum algorithm for Monte Carlo estimation. Still, the present work offers a polynomial speedup with respect to those results. Furthermore, their algorithms assume that the spectra of the matrix follows a uniform distribution, i.e. that the singular values are all $\Theta(1)$, which is not the case for low-rank matrices, and it is seldom the case for matrices that are obtained from datasets [60].

Interestingly, the fastest classical algorithms are based on function approximation techniques other than Chebyshev approximation (like Gaussian quadrature, the Lanczos method, and the Cauchy integral [16, 17,
These algorithms seem to achieve better scaling in terms of the condition number. However, these techniques seem not to be easily amenable for being translated to the quantum domain.

1.2 Our contributions

We present new quantum algorithms to estimate the log-determinant, the von Neumann entropy, the trace of inverse, and the Schatten-$p$ norm (see theorems 15, 18, 21, 23). All the results are reported in Table 1. For each of the algorithm, we prove its runtime and give guarantees on the approximation error. We use the framework of singular value transformation technique, developed in [11, 12, 23, 40] and others.

We improve upon the methodology of the previous quantum algorithm for log-determinant and Schatten-$p$ norm, i.e. the work of [66] (for which we better analyze the runtime and study the variance of the estimator) and [65]. We show how their approach - based on sampling - can benefit from quantum Monte Carlo methods, leading to polynomial speedsups.

| Spectral sum          | Classical            | Quantum (This work) | Thm. |
|-----------------------|----------------------|----------------------|------|
| Log-determinant       | $\tilde{O}(\|A\|_0 \sqrt{n}/\epsilon^2)$ | $\tilde{O}(\mu \kappa /\epsilon)$ | Thm. 15 |
| Schatten-$p$ norm      | $\tilde{O}(\|A\|_{op} \sqrt{n}/\epsilon^2)$ | $\tilde{O}(\sqrt{2}n \mu (\kappa + p)/\epsilon)$ | Thm. 18 |
| von Neumann entropy   | $\tilde{O}(\|A\|_{\kappa} \sqrt{n}/\epsilon^2)$ | $\tilde{O}(\mu^2 \kappa n /\epsilon)$ | Thm. 21 |
| Trace of inverse      | $\tilde{O}(\|A\|_0 \sqrt{n}/\epsilon^2)$ | $\tilde{O}(\mu^2 \kappa /\epsilon)$ | Thm. 23 |

Table 1: Comparison of classical/quantum algorithms for estimating different quantities of spectral sums. The classical algorithms for Schatten-$p$ norms, and trace of inverse, has been put forward in [28], and the algorithm for log-determinant comes from [28, 29]. The algorithm for the von Neumann entropy has been proposed in [38]. All the quantum algorithms assume to have quantum access to the matrix $A$. Quantum access to the matrix $A$ can be obtained with a preprocessing time that takes $O(\|A\|_0)$, as we detail in section 1.4. The algorithm for von Neumann entropy returns an absolute estimate, the other algorithms return a relative estimate.

1.3 Preliminaries and notation

We assume a basic understanding of quantum computing, and we recommend Nielsen and Chuang [50] for an introduction to the subject. A qubit is a mathematical representation of a quantum mechanical object as a $l_2$-normalized vector of length 2 on $\mathbb{C}^2$. The state of a $d$-qubit system (a register of a quantum computer) is the tensor product of $d$ single qubits: a unit vector $|x\rangle \in \mathbb{C}^{2^d}$. With log $n$ qubits we describe a quantum state $|\psi\rangle = \sum_i^2 \alpha_i |i\rangle$ with $\sum_i^2 |\alpha_i|^2 = 1$. The values $\alpha_j$ are called the amplitudes of the base state $|j\rangle$, where $|j\rangle$ represents the $j^{th}$ vector in the standard basis. For a vector $v \in \mathbb{R}^n$, we define $|v\rangle = \frac{1}{\sqrt{\|v\|}} \sum_{j \in [n]} v_j |j\rangle$.

The evolution of a quantum system is described by unitary matrices. A matrix $U$ is said to be unitary if $UU^\dagger = U^\dagger U = I$. It follows that unitary matrices are norm-preserving, and thus can be used as suitable mathematical description of pure quantum evolutions.

For a matrix $A = (a_{ij})_{n \times n} \in \mathbb{R}^{n \times n}$ we write $A = U \Sigma V^\dagger = \sum_{i=1}^n \sigma_i u_i v_i^\dagger$ as its singular value decomposition, where $\sigma_i$ are the singular values and $u_i, v_i$ its left and right singular vectors respectively. We use $\lambda_i$ to denote its eigenvalues. We assume that the singular values are sorted such that $\sigma_1$ is the biggest and $\sigma_n$ is the smallest. In this paper, we will use the following matrix norms:

- $\|A\|_0$ is the number of non-zero elements of the matrix $A$,
- $\|A\|_\infty$ is the biggest singular value of $A$,
- $\|A\|_F = \sqrt{\sum_{i,j=1}^n |a_{ij}|^2} = \sqrt{\sum_{i=1}^n \sigma_i^2}$ is the Frobenius norm,
\begin{itemize}
  \item $s_p(A) = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|^p$.
  \item $\|A\|_p = (\sum_i \sigma_i^p)^{1/p}$ is the Schatten-$p$ norm.
\end{itemize}

With $s$ we denote the sparsity, that is, the maximum number of non-zero elements of the rows. With $\kappa(A)$ we denote the condition number of $A$, that is, the ratio between the biggest and the smallest non-zero singular values. We also define

$$\mu(A) = \min_{p \in [0,1]} \left\{ \|A\|_p , \sqrt{s_2p(A)s_{2(1-p)}(A^T)} \right\}.$$  

(2)

**Remark 2.** When it makes no confusion, we will simply denote $\kappa(A)$ and $\mu(A)$ as $\kappa$ and $\mu$ respectively.

The singular value transformation is a technique comprehensively studied in [11, 23]. We refer to these two papers for an introduction about the subject. It is based on the definition of block-encoding of a matrix, i.e. a way to embed a matrix $A$ into the top-left part of a unitary matrix $U$.

**Definition 3** (Block-encoding). Suppose that $A$ is an $p$-qubit operator, $\alpha, \epsilon \in \mathbb{R}^+$ and $q \in \mathbb{N}$. Then we say that the $(p + q)$-qubit unitary $U$ is an $(\alpha, q, \epsilon)$-block-encoding of $A$, if:

$$\|A - \alpha((0^\otimes q \otimes I)U((0^\otimes q \otimes I))\| \leq \epsilon.$$  

**Lemma 4** (Constructing 1-block-encoding). Assume to have quantum access to a symmetric matrix $A \in \mathbb{R}^{n \times n}$ such that $\|A\| \leq 1$. For $\epsilon > 0$, there is a quantum circuit $V$ that implements a $(1, 1 + \log(n/\epsilon), \epsilon)$-block-encoding of $A$ in time $O(\mu/\epsilon)$.

**Theorem 5** (Polynomial eigenvalue transformation of arbitrary parity [23]). Suppose that $U$ is an $(\alpha, q, \epsilon)$-encoding of a Hermitian matrix $A$. If $\nu \geq 0$ and $P_\mathbb{R} \subseteq \mathbb{R}[x]$ is a degree-$d$ polynomial satisfying that for all $x \in [-1,1]$: $|P_\mathbb{R}(x)| \leq 1/2$. Then there is a quantum circuit $U$, which is an $(1, q + 2, 4\sqrt{\epsilon/\alpha + \nu})$-encoding of $P_\mathbb{R}(A/\alpha)$, and consists of $d$ applications of $U$ and $U^\dagger$ gates, a single application of controlled-$U$ and $O((q + 1)d)$ other one- and two-qubit gates. Moreover we can compute a description of such a circuit with a classical computer in time $O(\text{poly } d, \log(1/\nu))$.

To perform singular value transformation on the matrices of our interest, we need to have polynomial approximations of some functions.

**Lemma 6** (Efficient approximation of monomials on $[-1, 1]$ [54]). For positive integer $s,d$, there exist an efficiently computable polynomial $E_{s,d}(x) \in \mathbb{R}[x]$ of degree $d$ such that:

$$\sup_{x \in [-1,1]} |E_{s,d}(x) - x^s| \leq 2e^{-d^2/2s}.$$  

**Lemma 7** ([22, Lemma 11]). Let $\beta \in (0, 1]$, $\epsilon \in (0, 1/2)$. Then there exists a polynomial $\tilde{S}$ of degree $O(\frac{1}{\beta} \log(\frac{1}{\epsilon}))$ such that $|S(x) - \log(x) - 2\log(2\sqrt{e/\beta})| \leq \epsilon$ for all $x \in [\beta, 1]$, and $|S(x)| \leq 1/2$ for all $x \in [-1, 1]$.

**Lemma 8** ([12, 23]). Let $\epsilon, \delta \in (0, 1/2)$. Then there is a polynomial $\tilde{V}$ of degree $O(\frac{1}{\delta} \log(\frac{1}{\epsilon}))$ such that $|\tilde{V}(x) - 3\delta/8x| \leq \epsilon$ on the domain $[-1,1] \setminus [-\delta, \delta]$, moreover $|\tilde{V}(x)| \leq 1/2$ for all $x \in [-1,1]$.

**Lemma 9**. Let $\beta \in (0, 1]$, $\eta \in (0, 1/2)$. Then there exists a polynomial $\tilde{P}$ of degree $O(\frac{1}{\beta} \log(\frac{1}{\eta}))$ such that:

$$\forall x \in [\beta, 1] : |\tilde{P}(x) - \sqrt{x/3}| \leq \eta,$$

moreover $|\tilde{P}(x)| \leq 1/2$ for all $x \in [-1, 1]$.

### 1.4 Quantum access to classical data

In this work along with a fully-fledged quantum computer, we also assume to have access to a quantum memory (called QRAM), i.e. a device that allows a user to store classical data, which can answer queries in quantum superposition. In the QRAM model - before running the quantum algorithm - we pre-process the data so to construct a classical data structure, enabling quantum access to the data. The preprocessing takes linear time in the size of the data. To build quantum access for a matrix $M \in \mathbb{R}^{n \times m}$ the runtime will be $O(nm \log(mn))$. To stress more the fact that we are linear in the effective number of elements contained in the matrix (which can often be sparse), we often write this runtime as $\tilde{O}(\|A\|_0)$. This computational model is better formalized in the following definition.
Definition 10 (QRAM model [37]). An algorithm in the QRAM data structure model that processes a data-set of size $m$ has two steps:

1. A pre-processing step with complexity $\tilde{O}(m)$ that constructs efficient QRAM data structures for storing the data.

2. A computational step where the quantum algorithm has access to the QRAM data structures constructed in step 1.

The complexity of the algorithm in this model is measured by the cost for step 2.

When the data we want to access in a quantum algorithm is a matrix it is common to adopt the following model. The two model that follows are often the model of choice when working with non-dense graphs and matrices.

Definition 11 (Oracle access to a matrix). Let $A \in \mathbb{R}^{n \times n}$, there is an oracle that allows performing the mapping $|j,k,z\rangle \mapsto |j,k,z \oplus a_{j,k}\rangle$.

Definition 12 (Adjacency list access to a matrix). Let $A \in \mathbb{R}^{n \times n}$, and $d_{\text{max}}$ the maximum number of non-zero elements in the rows of $A$. There is an oracle that allows performing the mappings $|j,z,b\rangle \mapsto |j,z,b \oplus d_j\rangle$, where $d_j \leq d_{\text{max}}$ is the number of non-zero elements in row $A_j$ and $|j,l,b\rangle \mapsto |j,l,b \oplus \nu(j,l)\rangle$, for $l \leq d_j$, where $\nu(j,l)$ is the $l$-th nonzero entry of the $j$-th column of $A$.

Combined, the oracle access to $A$ and the adjacency list access makes the so-called quantum general graph model. Using either of the two models, it is possible to create quantum access to a matrix $A$.

Definition 13 (Quantum access to a matrix [11,23,35]). Let $A = (a_{ij}) \in \mathbb{R}^{d \times n}$, and $a_i$ be the $i$-th row of $A$. A quantum access to $A$ is a data structure such that, a quantum algorithm with access to it can perform the following unitaries in time $O(\text{polylog}(d))$:

1. $|i\rangle|0\rangle \rightarrow |i\rangle|a_i\rangle$ for $i \in [n]$.

2. $|0\rangle \rightarrow \frac{1}{\|A\|_F} \sum_{i \in [n]} \|a_i\| |i\rangle$.

The importance of this model is the following. Some datasets our society is producing are big enough such that it is only feasible to run linear time algorithms on them. Super-linear computations (like most linear-algebra based ML algorithms) are too computational expansive, as the size of the data is too big. Under this model, the cost of the computation using quantum hardware is given by the time of the preprocessing, where we construct the quantum access, plus the runtime of the quantum algorithm. The advantage of a quantum computer is to remove the dependence on the size of the dataset in the runtime of the algorithm. The price to pay is the additive cost to preprocess the data and create the data structure needed for quantum access. Let’s do an example. For estimating of the log-determinant, the best classical algorithm has a runtime of $O(\|A\|_0 \times \text{poly}(\kappa(A), 1/\epsilon))$. In the quantum case, the runtime of the whole data processing is $O(\|A\|_0 \log(\|A\|_F) + \text{poly}(\kappa(A), \epsilon^{-1}, \log(n)))$, which consist in $\tilde{O}(\|A\|_0)$ time for creating quantum access (and can be performed when the data is received) and the runtime of the quantum algorithm, which we show to be $O(\text{poly}(\kappa(A), \mu(A), \epsilon^{-1}, \log(n)))$. As the procedure to create quantum access is computationally easy to implement, (it requires only a few passes over the dataset) a quantum data analysis should be considerably faster than the classical procedure. It is clear that, even if the scaling of the quantum algorithm is sub-linear in the data (it is often, in fact, poly-logarithmic in $n$), if we consider in the runtime of the procedure also the time to build quantum access we “lose” the exponential gap between the classical and the quantum runtime. Nevertheless, the overall computational cost should still largely favor the quantum algorithm.

Will also assume that the matrix on which we have quantum access has been scaled by a number $\alpha$ such that the spectral norm is bounded, i.e. $\|A\| \leq 1$. This assumption can be easily satisfied, once quantum access for $A$ has been built. For instance, one can use [37, Algorithm 4.3, Proposition 4.8] to estimate $\|A\|$ with relative error, or $\kappa(A)$ with additive error in time $O(\frac{\|A\|_F \log(1/\epsilon)}{\|A\|_F})$. We assume that this procedure is done immediately after having built quantum access (which we recall requires $\tilde{O}(\|A\|_0)$) so the cost of this operation can be subsumed into the cost of creating quantum access to $A$. Once the matrix has been properly
scaled, we can update the data structure that we use for quantum access. As a final remark we anticipate that in some of the following algorithms, it will be convenient to assume quantum access to sub-normalized matrices, as in [11, Lemma 5], and [41] where \( \|A\| \leq 1 \). Again, this assumption can be easily satisfied by dividing the matrix by twice its biggest singular value before creating the data structures that allow quantum access.

As anticipated, in the following manuscript we will use quantum access to a matrix \( A \), i.e. definition 13 to build block-encodings as in definition 3. Using quantum access to a matrix, we can build a \((\mu(A), \log n, 0)\)-block-encoding, where the function \( \mu(A) \) is specified in definition 2. All the theorems presented here can be generalized, (as we do in theorem 15), where we assume to have a generic \((\alpha, q, \epsilon)\)-block-encoding of \( A \), for an appropriate choice of \( \epsilon \), and some \( \alpha \geq 1 \). This is standard practice in literature, see for example [36, 57]. We will also conflate the numbers of queries to the oracle that gives quantum access to a given matrix with the time complexity of the algorithm, as for this algorithms, the two quantities coincide. As an example, we leave the statement of theorem 15 in terms of queries to the oracle that produces the block-encoding.

2 Quantum algorithms for spectral sums

2.1 Proof techniques overview

The general idea of our quantum algorithms for spectral sums is to exploit the fact that the trace of a square matrix is equal to the sum of its eigenvalues. Thus, we perform trace estimation of a suitably created matrix which we manipulate with singular value transformation or any technique that allows us to apply a function to its spectra. The procedure is the following:

- Use quantum access to the matrix to obtain a unitary that encodes the matrix \( A \).
- Perform singular value transformation for the function of choice on the representation of \( A \).
- Use a suitable quantum trace estimation subroutine to estimate the trace of the transformed matrix \( f(A) \).

This procedure shares some similarities with the approach used in quantum algorithms used in property testing [22]. Using quantum access from quantum accessible data structure we have a \((\mu, \log n, 0)\)-block-encoding of a matrix. In fact, in the original statement of the theorem for the construction of a block-encoding from quantum accessible data structures, (i.e. [23, Lemma 48]), the authors build a \((\mu, \log n, \text{polylog}(\epsilon))\)-block-encoding, where the polylogarithmic error comes from the error in the approximation of the matrix entries \( a_{ij} \) with a certain number of bits of precision, which we assume to be sufficient to represent the entries of the matrix \( A \).

Note that, using singular value transformation, i.e. theorem 5, for a function \( f \) on a block-encoding with normalization factor \( \mu \), will return a block-encoding of \( f(A/\mu) \). For some of the problems discussed below, it is not convenient to obtain \( S_f(A) \) from \( S_f(A/\mu) \), as the normalization factor \( f(\mu) \) will appear in the runtime of the quantum algorithm. In this case, it is better to apply the singular value transformation to a \((1, q, \epsilon)\)-block-encoding of \( A \) (for \( \|A\| \leq 1 \)), which we show how to obtain using lemma 4) for matrices for which we have quantum access. Using the block-encoding of \( A \) obtained from the lemma 4 will generically have worse dependence on the error \( \epsilon \), but will help to keep the dependence on \( \mu \) bounded.

2.2 Log-determinant

An important special case of spectral sum is the log-determinant. The log-determinant is used in many different research areas, like Gaussian processes, Gaussian graphical models (also known as Markov random fields) [52, 53], and in tasks such as model selection, and model inference. The log-determinants also appears in Bayesian machine learning problems, as the computation of Bregman divergences [13]. Remark that in Gaussian graphical model the size of the matrix is quadratic in the number of variables used in the model.
**Definition 14** (Log-determinant of $A$). Let $A \in \mathbb{R}^{n \times n}$ be a real symmetric positive definite (SPD) matrix. Let $\sigma_1, \ldots, \sigma_n$ be the singular values of $A$. Then the log-determinant of $A$ is defined by:

$$\log \det(A) := \sum_{j=1}^{n} \log \sigma_j.$$ (3)

Observe that, while the determinant of a SPD matrix is always positive (because the eigenvalues are all positive), the log-determinant can be either positive or negative. Under the assumption that the singular values of the matrix lie in the interval $(0, 1]$, the log-determinant is always a negative quantity. In case $\|A\| \geq 1$, we define a matrix $A = A'/\alpha$ where $\alpha \geq \sigma_1(A')$. Then, we can recover the log-determinant of $A'$ as:

$$\log \det(A') = n \log(\alpha) + \log \det(A)$$ (4)

This intuition is better formalized in lemma 36 which we report from [7]. We will see that this assumption suits the model of quantum computation that we adopt. In this work, we also analyze the case when $\sigma_{\min} > 1$, and the case when $\sigma_1 > 1$ and $\sigma_{\min} < 1$, leading to a mixed sign problem of the logarithm. The classical algorithm of [7] runs in $O(\kappa^4 \|A\|_0/\epsilon)$, while the algorithm of [29] has a runtime of $O(\sqrt{\kappa} \|A\|_0/\epsilon)$.

**Algorithm 1** Log-determinant estimation using singular value transformations

**Require:** $(\alpha, q, \epsilon_1)$-block-encoding of a matrix $A \in \mathbb{R}^{n \times n}$ with $\|A\| < 1$, $\epsilon, \delta \in (0, 1)$.

**Ensure:** An estimate $|\log \det(A) - \log \det(A)| \leq \epsilon |\log \det(A)|$.

1. Set $\epsilon_2, \epsilon_3 \leq e^{\log(1/\|A\|)/6 \log(2\kappa \mu)}$.
2. Prepare the state

$$|\psi_0\rangle = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} |k\rangle |0\rangle.$$

3. Apply the block-encoding of $\tilde{S}(A/\mu)$ where $\tilde{S}(x)$ is the polynomial defined in lemma 7 with accuracy $\epsilon_3$, with precision $4\kappa \mu \sqrt{\epsilon_1 \mu} \log(1/\epsilon_1)$ to $|\psi_0\rangle$ to obtain:

$$|\psi_1\rangle = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} \tilde{S}(A/\mu) |k\rangle |0\rangle + |0^+\rangle.$$

4. Use inner product estimation subroutine with precision $\epsilon_2$ and failure probability $\delta$ to estimate $\langle \psi_0 | \psi_1 \rangle$, set the result as $L$.
5. Return $\log \det(A) = 2nL \log(2\kappa \mu) + n \log \mu$.

**Theorem 15** (SVT-based algorithm for log-determinant). Assume to have access to a unitary $U_A$ that is a $(\alpha, q, \epsilon_1)$-block-encoding of the SPD matrix $A \in \mathbb{R}^{n \times n}$ with $\|A\| < 1$. Let $\epsilon, \delta \in (0, 1)$, $\epsilon_1 \leq 2^2(\log \|A\|)^2/(\alpha \epsilon^2 \log^2(\kappa \alpha))$. Then Algorithm 1 returns the estimate $\log \det(A)$ such that $|\log \det(A) - \log \det(A)| \leq \epsilon |\log \det(A)|$ with probability at least $1 - \delta$, in $O(\alpha \kappa / \epsilon)$ calls to $U_A$ and $U_A^\dagger$.

**Proof.** Note that under the hypothesis $\|A\| < 1$ we have $|\log \det(A)| \geq n \log(1/\|A\|)$. We define as $\tilde{S}$ the polynomial approximation of the logarithm function (see lemma 7) with error $\epsilon_3$. Combined with theorem 5, we can create a $(1, q+2, 4\kappa \sqrt{\epsilon_1 \alpha} \log(1/\epsilon_1) + \nu)$-block-encoding of $\tilde{S}(A/\alpha)$ with circuit complexity $O(\alpha \kappa T)$. The description of the circuit can obtained in time $O(\text{poly}(d, \log(1/\nu)))$, where $d = O(\kappa \alpha \log(1/\epsilon_3))$ is the degree of the polynomial approximation we choose. As the runtime of this procedure is poly-logarithmic in $1/\nu$, we can take the error $\nu$ in the block-encoding as small as necessary, and it will not impact the runtime of the classical algorithm used to compute the circuit for the block-encoding. The polynomial approximation induces an error in the estimate of the log-determinant. We can bound this error, by analyzing the approximation of the singular values of the matrix $\tilde{S}(A/\alpha)$ as:

$$\left| \frac{\text{Tr}[\tilde{S}(A/\alpha)]}{n} - \frac{\log \det(A) - n \log \alpha}{2n \log(2\alpha \kappa)} \right| = \frac{1}{n} \left| \text{Tr}[\tilde{S}(A/\alpha)] - \sum_{j=1}^{n} \frac{\log(\sigma_j/\alpha)}{2 \log(2\alpha \kappa)} \right|.$$
The total cost of the algorithm is determined by the inner product estimation, which fails with probability \( \epsilon_3 \). The spectral sum for \( f \) is well-defined for non-square and non-symmetric matrices.

\[
\|
\begin{align*}
\sum_{j=1}^{n} \left| \tilde{S}(\sigma_j/\alpha) - \frac{\log(\sigma_j/\alpha)}{2 \log(2\kappa \alpha)} \right| \\
\leq \epsilon_3.
\end{align*}
\]

Note that, for \(|\psi_1\rangle\) and \(|\psi_2\rangle\) defined in Algorithm 1, we can check that:

\[
\langle \psi_0 | \psi_1 \rangle = \frac{1}{n} \sum_{k=1}^{n} (k | \tilde{S}(A/\alpha)|k) = \frac{\text{Tr}(\tilde{S}(A/\alpha))}{n}.
\]

The total error is given by three things: the error in the block-encoding of the polynomial approximation, i.e. theorem 5, which is \( 4\kappa \sqrt{1/\epsilon} \). The error \( \epsilon_2 \) in inner product estimation subroutine, that gives \( |L - \langle \psi_0 | \psi_1 \rangle| \leq \epsilon_2 \). And the error \( \epsilon_3 \) induced by the polynomial approximation on the trace, i.e. Equation (5). We set \( \epsilon_2, \epsilon_3 \leq \epsilon (\log 1/\|A\|)/(6 \log(2\kappa \mu)) \). These errors sums up additively, and thus we can use the triangle inequality to bound them.

\[
\left| \log \det(A) - \log \det(A) \right| = 2n \log(2\kappa \alpha) \left| \log \det(A) - n \log \alpha - L \right|
\]

\[
\leq 2n \log(2\kappa \alpha) \left| \log \det(A) - n \log \alpha - \frac{\text{Tr}(\tilde{S}(A/\alpha))}{n} \right|
\]

\[
+ 2n \log(2\kappa \alpha) \left| \frac{\text{Tr}(\tilde{S}(A/\alpha))}{n} - \langle \psi_0 | \psi_1 \rangle \right| + 2n \log(2\kappa \alpha) |\langle \psi_0 | \psi_1 \rangle - L|
\]

\[
\leq 2 \log(2\kappa \alpha) \left| \frac{\text{log det}(A)}{\log(1/\|A\|)} (\epsilon_3 + 4\kappa \sqrt{1/\epsilon} + \epsilon_2) \right| \log \det(A)]
\]

The total cost of the algorithm is determined by the inner product estimation, which fails with probability \( 1 - \delta \). The final runtime is \( \tilde{O}(\alpha \kappa \ell^4/\epsilon) \).

**Remark 16.** The case for \( \|A\| \leq 1 \) is already analyzed in the statement of the previous theorem, and here we consider the other two possible cases.

- In the case that \( \|A\| = 1 \), denote the multiplicity of the singular value 1 as \( m \). Then, we have that \( |\log \det(A)| \geq (n - m) \log(1/\sigma_{m+1}) \). Thus, in order to approximate \( \log \det(A) \) up to relative error \( \epsilon \), the complexity becomes \( \tilde{O}(\min_{\sigma_{m+1}} \log(1/\sigma_{m+1})) \).

- In the case where \( \|A\| > 1 \) and \( \sigma_n \leq 1 \), then we can define \( B = A/\alpha \) for some \( \alpha \geq \|A\| \). We thus obtain have \( \log \det(B) = \log \det(A) - n \log \alpha \). With Algorithm 1, we can approximate \( \log \det(B) \) up to precision \( \epsilon \). Thus, we can derive an approximation of \( \log \det(A) \) up to the same precision in cost \( \tilde{O}(\mu \kappa /\epsilon) \). But in this case, it is not possible to transform it into a relative error because of the mixed-sign for the logarithm of the singular values.

### 2.3 Schatten-\( p \) norm

The spectral sum for \( f(x) = x^p \) will allow us to recover the Schatten \( p \)-norm a matrix. Note that the Schatten-\( p \) norm is also well-defined for non-square and non-symmetric matrices.

**Definition 17** (Schatten-\( p \) norm). For a matrix \( A \in \mathbb{R}^{n \times n} \), and \( p \in \mathbb{N}^+ \), the Schatten-\( p \) norm \( \|A\|_p \) is defined as:

\[
\|A\|_p = \left( \sum_{i=1}^{\min(m,n)} \sigma_i^p \right)^{1/p}.
\]
When $p = 1$, it is also known as the nuclear or trace norm, and for $p = 2$ the Schatten-$2$ is the Frobenius norm. This is often used in matrix completion algorithms [48], in theoretical chemistry [26], differential privacy [31], and rank aggregation and collaborative ranking [42]. Furthermore, Schatten $p$-norms are often used in convex relaxations for rank-constrained optimization [49], and in image processing [43,63].

There are quantum algorithms for estimating the Schatten-$p$ norms. The paper [9] focus on a different model for the estimation of Schatten-$p$ norms (namely, the work in the DQC1 model, a restricted model of quantum computation), and they assume that $p, 1/e = O(\text{poly} \log n)$. Therefore, we believe it is unfair to compare their result with our, as the model is radically different. Another quantum algorithm for estimating Schatten-$p$ norms is due to [65]. The algorithm is similar in spirit to the quantum algorithm for the log-determinant by [66], and sample from the uniform distribution of singular values and perform the rest of the computation classically. Because of sampling technique employed there, the algorithm has an dependence on the precision of $O(e^{-3})$, and further depends quadratically on the Lipshitz constant $K_p$ of the function $\chi^p$ in the domain $[0,\sigma_{\text{max}}]$.

To our knowledge, the fastest classical algorithm for estimating the Schatten-$p$ norms [28, Theorem 4.5] has complexity $O(||A||_p^\text{op}/c^2)$, and has no assumption on $||A||$. Without loss of generality, we can assume that $||A|| < 1$. Thanks to the linearity of the norm, for any $c \in \mathbb{R}$, we have $||cA||_p = c||A||_p$. So if we can approximate $||cA||_p$ up to relative error $\epsilon$, we can also obtain an $\epsilon$-relative approximation of $||A||_p$. Note that a fast quantum algorithm for estimating the Schatten-$2$ norm is lemma 32, as $\text{Tr}[A^T A] = ||A||_F$, which can be seen as a special case of this algorithm.

**Theorem 18** (Algorithm for estimating Schatten-$p$ norms). Assume to have quantum access to a matrix $A \in \mathbb{R}^{m \times n}$ such that $||A|| < 1$. Then for any $\epsilon > 0$, $p \in \mathbb{N}^+$, there is a quantum algorithm that computes an $\epsilon$-relative approximation of the Schatten-$p$ norm of $A$ in time $O(\mu(\kappa + p)\sqrt{n2^p}/\epsilon)$.

**Proof.** Denote $B = A^T A$, then $||A||_p^p = \text{Tr}[B^{p/2}]$. Suppose that $p = 4q + r$, where $r \in \{0,1,2,3\}$. The basic idea of our quantum algorithm is to apply the trace estimation procedure of lemma 32 to approximate $\text{Tr}[B^{p/2}] = \text{Tr}[(B^{r/4})^q]$. To use lemma 32, we first need a block-encoding of $B^{r/4}$. From quantum access to $A$ we build a $(\mu, \log n, 0)$-block-encoding of $A$, and we build a $(1,2+2\log n, 0)$-block-encoding of $B/2$ by lemma 27 in time $O(\mu n)$. The block-encoding of $B^{r/4}$ can be constructed by theorem 5, and the block-encoding of $B^{r/4}$ can be constructed by lemma 28 for implementing positive powers of block-encodings.

First, we focus on the construction of the block-encoding of $B^q$. We set $f(x) = x^q/2$. By theorem 5, we can construct an $(1, 4+2\log n, \nu)$-block-encoding of $f(B/2) = B^q/2^{q+1}$ in time $O(\mu n)$. Here we can choose $\nu$ as small as we want since it appears only as logarithmic term in the complexity of the classical algorithms needed to create the quantum circuit. Also, note that the application of a monomial function add no error to the block-encoding.

Now we construct the block-encoding of $B^{r/4}$ by using lemma 28 with error $\epsilon_1$. We can create a $(1, 2+2\log n + O(\log(1/\epsilon_1)), \epsilon_1)$-block-encoding of $(B/2)^{r/4}/2 = B^{r/4}/2^{1+r/4}$ in time $O(\mu n)$.

We compose now the two block-encodings using the composition of preamplified block-encodings, i.e. lemma 27. We have a $(1, 6+4\log n + O(\log(1/\epsilon_1)), \nu + \epsilon_1)$-block-encoding of $B^{q/2}/2^{2q+1/4}$ in time $O(\mu(\kappa + q))$.

We choose $\nu, \epsilon_1$ such that $\nu = O(\epsilon_1)\text{Tr}[B^{p/2}/2^{4+p/2}]/4n)$. Now we use the trace estimation subroutine of lemma 32, and we note that $\text{Tr}[B^{p/2}/2^4 + p/2] = \Omega(1/2^4 + p/2)$. Thus, in time $O(\mu(\kappa + q)\sqrt{n2^p}/\epsilon)$, we estimate an $S$ such that

$$|S - \text{Tr}[B^{p/2}/2^{4+p/2}]| \leq \epsilon\text{Tr}[B^{p/2}/2^{4+p/2}].$$

As we have a relative error estimate, this also means that, by taking $\alpha^p = 2^{4+p/2}$, we have $|\alpha^p S - ||A||_p^p| \leq \epsilon||A||_p^p$. Recall that for $a, b \in \mathbb{R}$, we have that $(a^b - b^a) = (a - b)(\sum_{i=0}^b a^i b^{b-1-i})$. Thus we have:

$$|\alpha^{1/p} S - ||A||_p^p| = |\alpha^p S - ||A||_p^p| = \frac{|\alpha^p S - ||A||_p^p|}{\alpha^p - 1} = \frac{|\alpha^p S - ||A||_p^p|}{\alpha^{p-1} S^{(p-1)/p} + \alpha^{p-2} S^{(p-2)/p}||A||_p + \cdots + ||A||_p^{p-1}} \leq \epsilon||A||_p^p.$$

This completes the proof.

**Remark 19.** We can use lemma 6 to obtain a polynomial approximation of the monomial $x^p/2$ of degree $\sqrt{2p}\log(1/\epsilon')$. This will introduce an error that can be chosen to be $\epsilon' \leq \epsilon\text{Tr}[B^{p/2}/2^{4+p/2}]/8n$ and incurring only in a polylogarithmic increase in the runtime.
2.4 Von Neuman entropy

If we compute \( S_f(A) \) for \( f(x) = -x \log x \), then we are estimating the von Neumann entropy. In graph theory, the von Neumann entropy is a spectral complexity measure that has applications in complex networks analysis and pattern recognition [30, 45]. In quantum physics, it quantifies the departure of the quantum system from a pure state [6]. The von Neumann entropy is also important in feature selection [4], financial data analysis [10], and genomic data [1]. The current best classical algorithm [38, Theorem 2] has complexity \( \tilde{O}(\| A \|_0 \kappa / \epsilon^2) \). There is a rich literature for quantum algorithms for estimating von Neumann entropy and other entropies, among the many we cite [39, 56], and [22], whose approach is the most similar to our.

**Definition 20** (von Neumann entropy of a density matrix). For a density matrix \( A = \sum_{i=1}^{n} \lambda_i |\psi_i\rangle \langle \psi_i| \in \mathbb{R}^{n \times n} \) the von Neumann entropy of \( A \) is defined as:

\[
H(A) = -\text{Tr}[A \log A] = - \sum_{i=1}^{n} \lambda_i \log \lambda_i. \tag{7}
\]

In the following theorem, when we say quantum access to a density operator, we mean that we can create a block-encoding of a density matrix. This assumption can be satisfied in two ways: either by storing the matrix in a QRAM-like data structure, or by assuming to have access to a unitary matrix that produces a state that is the purification of a density matrix, as is described in lemma 29 in the supplementary material.

**Theorem 21** (Algorithm for estimating von Neumann entropy). Assume to have quantum access to density operator \( A \in \mathbb{R}^{n \times n} \). Then for any \( \epsilon > 0 \), there is a quantum algorithm that computes an \( \epsilon \)-absolute approximation of \( H(A) \) with high probability in time \( \tilde{O}(\mu^2 \kappa n / \epsilon) \).

**Proof.** We can use again the polynomial \( \tilde{S}(x) \) defined in lemma 7 for approximating the logarithm function up to error \( \epsilon_1 \). Then the function \( f(x) = -x (\log x) / (2 \log (2/\beta)) \) is approximated on the interval \([\beta, 1]\) by \( P(x) = -x \tilde{S}(x) \) with error \( \epsilon_1 \), where we take \( \beta = 1 / \mu \kappa \). The degree of \( P(x) \) is \( O(\kappa \mu \log (1 / \epsilon_1)) \). Note that \( |P(x)| \leq 1 / 2 \), so it satisfies the requirements of theorem 5. With it, we can create a \((1, 2 + \log n, 0)\)-block-encoding of \( P(A/\mu) \) in time \( \tilde{O}(\kappa \mu) \). We use this block-encoding in the trace estimation subroutine with absolute error using lemma 31, which returns an estimate

\[
\left| \text{Tr}[P(A/\mu)] - \text{Tr}[P(A/\mu)] \right| \leq \frac{\epsilon}{4 \mu \log (2 \mu \kappa)}
\]

in time \( \tilde{O}(\kappa \mu^2 n / \epsilon) \). Note that, for \( \beta = 1 / \mu \kappa \),

\[
\text{Tr}[f(A/\mu)] = - \frac{1}{2 \log (2 \mu \kappa)} \sum_{i=1}^{n} \frac{\sigma_i}{\mu} \log \frac{\sigma_i}{\mu} = \frac{H(A)}{2 \mu \log (2 \mu \kappa)} + \frac{\log \mu}{2 \mu \log (2 \mu \kappa)}.
\]

This means that we can obtain our quantity as \( H(A) = 2 \mu \log (2 \mu \kappa) (\text{Tr}[f(A/\mu)]) - \log \mu \). From the polynomial approximation of lemma 7,

\[
\left| \text{Tr}[f(A/\mu)] - \text{Tr}[P(A/\mu)] \right| \leq \sum_{i=1}^{n} \frac{\sigma_i}{\mu} \left| \log (\sigma_i / \mu) \right| - \tilde{S}(\sigma_i / \mu) \leq \sum_{i=1}^{n} \frac{\sigma_i \epsilon_1}{\mu} = \frac{\epsilon_1}{\mu}.
\]

So our estimate of \( H(A) \) is defined as \( \bar{H}(A) = 2 \mu \log (2 \mu \kappa) \left( \text{Tr}[P(A/\mu)] \right) - \log \mu \).

The total error in the procedure accumulates additively and thus can be bounded as follow:

\[
\left| H(A) - \bar{H}(A) \right| = 2 \mu \log (2 \mu \kappa) \left| \text{Tr}[f(A/\mu)] - \text{Tr}[P(A/\mu)] \right| \leq 2 \mu \log (2 \mu \kappa) \left( \left| \text{Tr}[f(A/\mu)] - \text{Tr}[P(A/\mu)] \right| + \left| \text{Tr}[P(A/\mu)] - \text{Tr}[P(A/\mu)] \right| \right) \leq 2 \mu \log (2 \mu \kappa) \left( \frac{\epsilon_1}{\mu} + \frac{\epsilon}{4 \mu \log (2 \mu \kappa)} \right).
\]

To make sure the above error is bounded by \( \epsilon \), it suffices to choose \( \epsilon_1 = \epsilon / 4 \log (2 \mu \kappa) \). The total runtime of the above algorithm is \( \tilde{O}(\kappa \mu^2 n / \epsilon) \). \( \Box \)
2.5 Matrix inverse

The trace of a matrix inverse is the spectral sum for the function $f(x) = 1/x$. Computing this quantity has wide applications, especially in the study of lattice quantum chromodynamics [55], fractals [62], generalized cross validation [24] and uncertainty quantification [14].

**Definition 22** (Trace of inverse). For an SPD matrix $A \in \mathbb{R}^{n \times n}$ the trace of the inverse of $A$ is defined as:

$$I(A) = \text{Tr}[A^{-1}] = \sum_{i=1}^{n} \frac{1}{\sigma_i}.$$

Note that for any nonzero $\alpha$, we have $I(\alpha A) = I(A)/\alpha$. Thus, if we can approximate the trace of a matrix inverse of a scaled matrix $I(A/\|A\|)$ up to relative error $\epsilon$, we can also obtain an $\epsilon$-relative approximation of the normalized quantity $I(A)$.

A classical algorithm [28, Theorem 4.3] to solve this problem has complexity $O(\|A\|_0 \sqrt{n}/\epsilon^2)$. Another classical algorithm, which uses Stochastic Lanczos Quadrature [59] has a similar runtime, but converges twice as fast as the algorithms based on the Chebyshev expansion.

**Theorem 23** (Algorithm for estimating the trace of the inverse). Assume to have quantum access to a (non-singular) SPD matrix $A \in \mathbb{R}^{n \times n}$ such that $\|A\| \leq 1$. Then for any $\epsilon > 0$, there is a quantum algorithm that computes a $\epsilon$-relative approximation of $\text{Tr}[A^{-1}]$ with high probability, in time $O(\mu \kappa^2/\epsilon)$.

**Proof.** Under the hypothesis that $\|A\| \leq 1$ we observe that $I(A) \geq n$. From the quantum access to $A$, we can obtain an $(\mu, \log n, 0)$-block-encoding of $A$. We perform singular value transformation (i.e., theorem 5) along with the polynomial approximation $\tilde{V}(x)$ (see lemma 8) of the inverse function $f(x) = 3\delta/8x$ on the interval $[-1, 1]$, with error $\epsilon_1$, δ = 1/μκ, and so the degree of $\tilde{V}$ is $O(\mu \kappa \log(2n/\epsilon))$. The singular value transformation gives us a $(1, 2 + \log n, \nu)$-block-encoding of $\tilde{V}(A/\mu)$, where $\nu$ can be set as small as possible. We use this block-encoding in the trace estimation subroutine (i.e. lemma 31) with absolute error $n\epsilon_2$, obtaining an estimate $T$ such that

$$\left| \text{Tr}[\tilde{V}(A/\mu)] - T \right| \leq n\epsilon_2.$$

The circuit complexity of this operation is $O(\mu \kappa / \epsilon_2)$. From the polynomial approximation of lemma 8 where we set $\delta = 1/\mu \kappa$, we have

$$\left| \text{Tr}[\tilde{V}(A/\mu)] - \frac{3}{8 \mu \kappa} I(A/\mu) \right| \leq \sum_{i=1}^{n} \left| \tilde{V}(\sigma_i/\mu) - \frac{3}{8 \mu \kappa \sigma_i} \right| \leq n\epsilon_1.$$

So we define our estimate as $I(A) = 8 \mu \kappa T / 3$. The error analysis is the following:

$$\left| I(A) - I(A) \right| \leq \left| I(A) - \frac{8 \mu \kappa}{3} \text{Tr}[\tilde{V}(A/\mu)] \right| + \frac{8 \mu \kappa}{3} \left| \text{Tr}[\tilde{V}(A/\mu)] - T \right| \leq \frac{8 \mu \kappa (\epsilon_1 + \epsilon_2)}{3} \leq \frac{8 \mu \kappa (\epsilon_1 + \epsilon_2)}{3} I(A).$$

To obtain a relative error, we set $\epsilon_1 = \epsilon_2 = 3\epsilon / 16 \mu \kappa$. The complexity then becomes $O(\mu^2 \kappa^2 \|A\|/\epsilon)$.

3 Conclusions and future works

In this work, we show how to use quantum singular value transformation and quantum trace estimation subroutines to estimate most of the spectral quantities of interest. In the theorems presented in this work, we assume quantum access to a matrix, from which we can build a $(\mu, \log n, 0)$-block-encoding. This can be generalized - as we do in theorem 15 - to assume a $(\alpha, q, \epsilon)$-block-encoding.

Estrada index is perhaps a spectral sum that is not suitable to be estimated with our approach. This index was defined by Ernesto Estrada as a measure of the degree of folding of a protein [18], which has found applications in the study of protein functions and protein-ligand interactions [15]. Currently, it is...
also used in statistical thermodynamics [20,21] and network theory [19]. In [28, Theorem 4.4], they showed that the Estrada index can be approximated up to a relative error in cost $\tilde{O}(\|A\|\kappa/\epsilon^2)$. The Estrada index of a undirected simple graph $G$ of $n$ nodes is defined on its adjacency matrix $A$ of $G$ as $E(A) = \sum_i^n e^{\lambda_i}$. Using the framework of singular value transformation to estimate this quantity poses some issues. First, as we need that $\|A\| \leq 1$, we can only estimate some normalized version of $E(G)$, as we can estimate $E_N(A) = \sum_i^n e^{\lambda_i}/\lambda_{i1}$. It is simple to get rid of the normalization factor of $\mu$ by working with block-encoding where $\mu = 1$, and we show how to build one in lemma 4. Moreover, as the Estrada index is defined on the eigenvalues (and not on the singular values), we cannot use the framework of singular value transformation, as there are often negative eigenvalues in adjacency matrices of graphs. To circumvent this issue we have two options. We could either use quantum signal processing techniques [40], which manipulates the eigenvalues of matrices, and thus keeps the sign information, or shift the spectrum of $A$ working with $B = A + \gamma I$ for a certain $\gamma$, which can be efficiently estimated using [37, Algorithm 4.3, Proposition 4.8]. A different option would be to work see the Estrada index as the sum of the number of all weighted closed walks of all lengths, where the number of walks of length $k$ is scaled by a factor of $1/k!$. In fact [33], for $n_k = \sum_i^N \lambda_i^k = \text{Tr}[A^k]$ we have that:

$$E(G) = \sum_{k=0}^{\infty} \frac{n_k}{k!} = \sum_{k=0}^{\infty} \sum_{i=1}^{N} \frac{\lambda_i^k}{k!} = \sum_{i=1}^{N} e^{\lambda_i}.$$  

Exploiting this intuition might lead to fast quantum algorithms for estimating the Estrada index.

Future works include the study of the applications of quantum algorithms for spectral sums. Some applications include the estimate of the log-determinant of covariance matrices, i.e. $\log \det(C^TC)$, counting the number of triangles in undirected graphs and the spanning trees of a graph, and the log-likelihood of covariance matrix estimator like the Tyler’s M-estimator.

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A Supplementary Material

Definition 24 (SVE Problem [37]). Let $A = \sum_{i \in [k]} \sigma_i |u_i\rangle \langle v_i|$ be the singular value decomposition of the matrix $A \in \mathbb{R}^{m \times n}$, where $k = \min(m, n)$. Let $\epsilon \in (0, 1)$. The singular value estimation (SVE) problem with accuracy $\epsilon$ is defined as: Given $|b\rangle = \sum_{i \in [k]} \beta_i |v_i\rangle$ to perform the mapping

$$\sum_{i \in [k]} \beta_i |v_i\rangle |0\rangle \mapsto \sum_{i \in [k]} \beta_i |v_i\rangle |\tilde{\sigma}_i\rangle,$$

such that $|\tilde{\sigma}_i - \sigma_i| \leq \epsilon$ for all $i \in [k]$ with probability at least $1 - 1/\text{poly}(n)$.

Lemma 25 (SVE Algorithm - [37, Theorem 4.4]). Let $A \in \mathbb{R}^{m \times n}$ be a matrix, for which we have quantum access. Let $\epsilon > 0$ be the precision parameter. Then there is a quantum algorithm with running time $O(\mu/\epsilon)$ that solves the SVE problem.

Lemma 4 (rephrased). Assume to have quantum access to a symmetric matrix $A \in \mathbb{R}^{n \times n}$ such that $\|A\| \leq 1$. For $\epsilon > 0$, there is a quantum circuit $V$ that implements a $(1, 1 + \log(n/\epsilon), \epsilon)$-block-encoding of $A$ in time $O(\mu/\epsilon)$.

Proof. We will show how to create a block encoding of $A$ with normalization factor equals 1. Remember that a $(\mu, q, \epsilon)$ block encoding of a matrix $A$ to a quantum state $|x\rangle$ means that:

$$\|A|x\rangle - \mu((0) \otimes I)U((0) \otimes |x\rangle)\| \leq \epsilon.$$

With quantum access to the matrix $A$, we can obtain an $(\mu, \log n, \epsilon)$-block-encoding of $A$, for some $\epsilon \geq 0$.

Let $A = \sum_{j=1}^{n} \sigma_j |u_j\rangle \langle u_j|$ be the SVD of $A$. For any state $|x\rangle = \sum_j \beta_j |u_j\rangle$, using SVE (i.e. Lemma 25) we can create $\sum_j \beta_j |u_j\rangle |\tilde{\sigma}_j\rangle$ in time $O(\mu/\epsilon)$, where $|\sigma_j - \tilde{\sigma}_j| \leq \epsilon$. Using a controlled rotation, and undoing the SVE, we can generate the state

$$\sum_j \beta_j \left( |\tilde{\sigma}_j 0^{t+1}\rangle + \sqrt{1 - |\tilde{\sigma}_j|^2} |1\rangle \right) |u_j\rangle =: |0^{t+1}\rangle \otimes \overline{A|x\rangle} + \text{orthogonal parts}.$$

In the previous state, the register $|0^{t+1}\rangle$ is made of $t = \log(1/\epsilon)$ qubits used to perform the phase estimation step of the SVE and 1 ancillary qubit to perform the controlled rotation. Since $|\sigma_j - \tilde{\sigma}_j| \leq \epsilon$ and $|u_j\rangle$ are orthogonal vectors, we have $\|A|x\rangle - \overline{A|x\rangle}\| \leq \epsilon$. Let $V$ the unitary that perform the steps up to Equation (9). Then, $\|A|x\rangle - ((0) \otimes I)V((0) \otimes |x\rangle)\| \leq \epsilon$. The unitary $V$ is thus a $(1, 1 + \log(n/\epsilon), \epsilon)$-block-encoding of $A$ with a gate complexity $O(\mu/\epsilon)$.

Theorem 26 (Combination of block-encodings [23]). Suppose that $U$ is a $(\alpha, a, \delta)$-block-encoding of a $q$-qubit operator $A$, and $V$ is a $(\beta, b, \epsilon)$-block-encoding of a $q$-qubit operator $B$. Then, considering the Hilbert space $\mathbb{C}^{2^q} \otimes \mathbb{C}^{2^q} \otimes \mathbb{C}^2$, successively applying $V$ to the first and third register, and $U$ to the first and second, yields an $(\alpha \beta, a + b, \alpha \epsilon + \beta \delta)$-block-encoding of $AB$.

If we have 2 (or more) sub-normalized block-encodings, we can combine them more efficiently. Based on the previous Theorem 26, we have the following lemma.

Lemma 27 (Product of preamplified block-encodings [11, Lemma 5]). Let $A_1 \in \mathbb{R}^{l \times m}, A_2 \in \mathbb{R}^{m \times n}$ such that $\|A_1\| \leq 1, \|A_2\| \leq 1$. For $i \in \{1, 2\}$, suppose $\alpha_i \geq 1$ and we have an $(\alpha_i, a_i, \epsilon_i)$-block-encoding of $A_i$ that can be implemented in time $O(T_i)$, then there is a $(1, a_1 + a_2 + 2, \epsilon_1 + \epsilon_2)$-block-encoding of $A_1 A_2 / 2$ that can be implemented in time $O(\alpha_1(q_1 + T_1) + \alpha_2(q_2 + T_2))$. 

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Lemma 28 (Implementing positive powers of Hermitian matrices [11, Lemma 10]). Let $c \in (0, 1], \kappa \geq 2$, and $H$ be a Hermitian matrix such that $I/\kappa \preceq H \preceq I$. Suppose that $\delta = o(\epsilon(\kappa \log^3(\kappa/\epsilon)))$, and we are given an $(\alpha, a, \delta)$-block-encoding of $H$ that is implemented in $O(T)$ elementary gates. Then for any $\epsilon$, we can implement a unitary that is a $(1, a + O(\log \log(1/\epsilon)), \epsilon)$-block-encoding of $H^c/2$ in cost $O(\alpha \kappa (a + T) \log^2(\kappa/\epsilon))$.

Lemma 29 (Block-encoding of density operators [23, Lemma 45]). Suppose that $\rho$ is an $s$-qubit density operator, $G$ is an $(a + s)$-qubit unitary that on the $\ket{0} \ket{0}$ input state prepares a purification $\ket{0} \ket{0} \mapsto \ket{\rho}$, s.t. $\Tr_a[\rho](\rho) = \rho$. Then $(G^\dagger \otimes I_a)(I_a \otimes \text{SWAP})(G \otimes I_a)$ is a $(1, a + s, 0)$-block-encoding of $\rho$.

Theorem 30 (Quantum amplitude estimation [8]). There is a quantum algorithm which takes as input one copy of a quantum state $\ket{\psi}$, a unitary transformation $U = 2 \ket{\psi} \bra{\psi} - I$, a unitary transformation $V = I - 2P$ for some projector $P$, and an integer $t$. The algorithm outputs $\tilde{a}$, an estimate of $a = \bra{\psi} P \ket{\psi}$, such that

$$|a - \tilde{a}| \leq \frac{2\pi \sqrt{a(1 - a)}}{t} + \frac{\pi^2}{t^2}$$

(10)

with probability at least $8/\pi^2$, using $U$ and $V$ $t$ times each.

Lemma 31 (Quantum trace estimation). Let $\epsilon \in (0, 1)$ and $A \in \mathbb{R}^{n \times n}$ be a SPD matrix with $\|A\| \leq 1$. Let $U$ be a $(\alpha, q, \epsilon/2)$ block-encoding of $A$ that is constructed in time $O(T)$. Then there is a quantum algorithm that returns $\Tr[A]$ with probability at least $2/3$ such that:

- $|\Tr[A] - \Tr[A]| \leq \epsilon \Tr[A]$ in time $O(\alpha n T/\epsilon)$.
- $|\Tr[A] - \tilde{\Tr}[A]| \leq \epsilon \Tr[A]$ in time $O(\alpha n T/\epsilon)$.

Proof. Denote the top-left corner of $U$ as $\tilde{A}$, then $\|A - \tilde{A}\| \leq \delta$. The algorithm is as follows. First, we apply $U$ to $\ket{\phi} = (1/\sqrt{n}) \sum_{i=1}^n \ket{i}$ to obtain $\ket{\psi} = A \ket{\phi} \ket{0} + \ket{\psi_i}$. Then we set up the state of the Hadamard test as follow:

$$\frac{1}{2} \ket{0}(\ket{\psi} + \ket{\phi, 0}) + \frac{1}{2} \ket{1}(\ket{\psi} - \ket{\phi, 0})$$

Since $\ket{\psi, \phi, 0}$ is $\Tr[\tilde{A}]/n$, the square of the amplitude of $\ket{0}$ equals $a := (1 + \Tr[\tilde{A}]/n)/2$. Finally, by amplitude estimation, we obtain $\tilde{a}$ such that $|a - \tilde{a}| \leq \epsilon/4a$ by choosing $t = 8\alpha n/\epsilon$ in Equation (10). The complexity of the above procedure is $O(Ta/\epsilon)$.

Since $\|A - \tilde{A}\| \leq \delta$, it follows that $|\Tr[A] - \alpha \Tr[\tilde{A}]| \leq \epsilon \Tr[A]$. Now set $\tilde{\Tr}[A] = n\alpha (2\tilde{a} - 1)$, then

$$|\Tr[A] - \tilde{\Tr}[A]| \leq |\Tr[\tilde{A}] - \alpha \Tr[A]| + |\Tr[A] - \alpha \Tr[\tilde{A}]| \leq \epsilon \Tr[A]$$

This gives the first claim. The second claim comes from the first one by setting the error as $\epsilon \Tr[A]/n$. \qed

Finding the trace of the product of two matrices is important in the context of SDPs (semi-definite programming), but it will be useful in spectral sums as well.

Lemma 32 (Trace estimation of product [25]). Let $U$ be a $(1, q, \delta)$-block-encoding of a matrix $B \in \mathbb{C}^{n \times n}$ that satisfies $\Tr[B^\dagger B] = \Omega(1)$. Let $0 \leq \epsilon \leq 1$ and assume $\delta \leq \epsilon \Tr[B^\dagger B]/4n$. A multiplicative $\epsilon$-approximation of $\Tr[B^\dagger B]$ can be computed using $O(T_U \sqrt{n}/\epsilon)$, where $O(T_U)$ is the complexity to implement $U$.

Lemma 33 (Distance / Inner Products Estimation [34]). Assume for a matrix $V \in \mathbb{R}^{n \times d}$ and a matrix $C \in \mathbb{R}^{k \times d}$ that the following unitaries $|i\rangle|0\rangle \mapsto |i\rangle|v_i\rangle$, and $|j\rangle|0\rangle \mapsto |j\rangle|c_j\rangle$ can be performed in time $T$ and the norms of the vectors are known. For any $\Delta > 0$ and $\epsilon > 0$, there exists a quantum algorithm that computes

$$|i\rangle|j\rangle|0\rangle \mapsto |i\rangle|j\rangle|d^2(v_i, c_j)|, \text{ where } |d^2(v_i, c_j) - d^2(v_i, c_j)| \leq \epsilon \text{ w.p. } \geq 1 - 2\Delta, \text{ or}$$

$$|i\rangle|j\rangle|0\rangle \mapsto |i\rangle|j\rangle|v_i, c_j|, \text{ where } |v_i, c_j - (v_i, c_j)| \leq \epsilon \text{ w.p. } \geq 1 - 2\Delta$$

in time $\tilde{O}(\|v_i\|_2 \|c_j\|_2 T \log(1/\Delta))$. 

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B Four quantum algorithms for the log-determinant

For the log-determinant we explored various methodologies for quantum algorithm design, which we report here. One reason why we investigate these algorithms is that we want to compare all the possible quantum algorithms to compute log-determinant and try to find the optimal technique to solve matrix problems. Our analysis provides further evidence that the block-encoding is a powerful and versatile framework for working with matrices.

The following algorithms are based on the following techniques: quantum singular value estimation (SVE), Taylor approximation, Chebyshev approximation and Monte Carlo sampling. The SVE algorithm seems the most naive one to compute log-determinant, and in fact it turns out to be the most inefficient one. The results can be observed in Table 2. All our algorithms are based on the following assumption.

| Quantum Algorithms                  | Complexity                        |
|-------------------------------------|-----------------------------------|
| SVT-based (Theorem 15)              | $\tilde{O}(\mu \kappa / \epsilon)$ |
| SVE-based (Theorem 35)              | $\tilde{O}(\mu \kappa^3 / \epsilon^2)$ |
| Taylor approximation (Theorem 38)   | $\tilde{O}(\mu \kappa^2 / \epsilon^2)$ |
| Chebyshev approximation (Theorem 41) | $\tilde{O}(\mu \kappa / \epsilon^2)$ |
| Quantum Monte Carlo (Theorem 46)    | $\tilde{O}(\mu \kappa / \epsilon^2)$ |

Table 2: Comparison of different quantum algorithms to estimate log-determinant.

Assumption 34. Let $A \in \mathbb{R}^{n \times n}$ by a SPD matrix such that $\|A\| \leq 1$ for which we have quantum access as in Definition 13.

Under the assumption that $\|A\| < 1$, we have $|\log \det(A)| \geq n \log(1 / \|A\|)$. In our algorithms below, it is more convenient to estimate the error up to $n \epsilon$. However with this simple observation, it can be changed into a relative error without so many influences on the complexity.

B.1 Singular Value Estimation

We start our series of quantum algorithms for the log-determinant using a pretty straightforward approach, i.e. using the quantum algorithm for singular value estimation (SVE). The SVE problem can be stated in a very general form (see Definition 24). However, in this following, we only focus on the special case of Hermitian matrices.

Theorem 35. Under assumption 34, algorithm 2 returns $\overline{\log \det(A)}$ such that $|\log \det(A) - \log \det(A)| < \epsilon |\log \det(A)|$ in time $\tilde{O}(\mu \kappa^3 / \epsilon^2)$.

Proof. We can rewrite the quantum state encoding the representation of $A$ (which we can create with quantum access to $A$) as follow:

$$|A\rangle = \frac{1}{\|A\|_F} \sum_{i,j=1}^{n} a_{ij} |i,j\rangle = \frac{1}{\|A\|_F} \sum_{j=1}^{n} \sigma_j |u_j\rangle |u_j\rangle.$$  

Starting from the state $|A\rangle$, we can apply SVE (see Lemma 25) to $|A\rangle$ up to precision $\epsilon_1$ to obtain

$$\frac{1}{\|A\|_F} \sum_{j=1}^{n} \sigma_j |u_j\rangle |u_j\rangle |\tilde{\sigma}_j\rangle,$$

where $|\tilde{\sigma}_j - \sigma_j| \leq \epsilon_1$. Since $\|A\| \leq 1$, using controlled operations, we can prepare

$$\frac{1}{\|A\|_F} \sum_{i=1}^{n} \sigma_j |u_j\rangle |u_j\rangle |\tilde{\sigma}_j\rangle \left( C \sqrt{-\frac{\log \tilde{\sigma}_j}{\tilde{\sigma}_j}} |0\rangle + |0^\perp\rangle \right),$$  

(11)

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**Algorithm 2** SVE-based quantum algorithm for the log-determinant

**Require:** Quantum access to the SPD matrix $A \in \mathbb{R}^{n \times n}$ such that $\|A\| \leq 1$. Choose $\epsilon \in (0,1)$, $\epsilon_1 = \epsilon / \kappa \log \kappa$ and $\epsilon_2 = \epsilon / \kappa^2 \log \kappa$.

**Ensure:** An estimate $|\|\log \det(A) - \log \det(A)\|| \leq n\epsilon$.

1. Prepare
   $$|A\rangle = \frac{1}{\|A\|_F} \sum_{i,j=1}^{n} a_{ij}|i,j\rangle.$$

2. Perform SVE by Lemma 25 up to precision $\epsilon_1$ and do control rotations to prepare
   $$\frac{1}{\|A\|_F} \sum_{j=1}^{n} \sigma_j |u_j\rangle |\bar{\sigma}_j\rangle \left( C \sqrt{\log \sigma_j \|\sigma_j\|} |0\rangle + |\perp\rangle \right),$$
   where $C = \min_j \bar{\sigma}_j / \sqrt{\log \sigma_j} \approx \sigma_{\min} / \sqrt{\log \sigma_{\min}} = 1 / \kappa \sqrt{\log \kappa}$.

3. Apply amplitude estimation to estimate the probability of $|0\rangle$ to precision $\epsilon_2$. Set the result as $P$.

4. Return $\frac{\log \det(A)}{\log \det(A)} = -\kappa^2 (\log \kappa) \|A\|^2_2 P$.

where $C = \min_j \bar{\sigma}_j / \sqrt{\log \sigma_j} \approx \sigma_{\min} / \sqrt{\log \sigma_{\min}} = 1 / \kappa \sqrt{\log \kappa}$. The probability of $|0\rangle$ is

$$P = \frac{C^2}{\|A\|^2_2} \sum_{j=1}^{n} \frac{\sigma_j^2}{\bar{\sigma}_j^2} \log \bar{\sigma}_j.$$

First, we do the error analysis. Note that

$$\left| \sum_{j=1}^{n} \frac{\sigma_j^2}{\bar{\sigma}_j^2} \log \bar{\sigma}_j - \sum_{j=1}^{n} \log \sigma_j \right| \leq \sum_{j=1}^{n} \left| \frac{\sigma_j^2}{\bar{\sigma}_j^2} \log \bar{\sigma}_j - \sum_{j=1}^{n} \frac{\sigma_j^2}{\bar{\sigma}_j^2} \log \sigma_j \right| + \sum_{j=1}^{n} \left| \frac{\sigma_j^2}{\bar{\sigma}_j^2} \log \sigma_j - \sum_{j=1}^{n} \log \sigma_j \right|$$

$$\leq \sum_{j=1}^{n} \frac{\sigma_j^2}{\bar{\sigma}_j^2} \left| \log \sigma_j - \log \bar{\sigma}_j \right| + \sum_{j=1}^{n} \left| \frac{\sigma_j^2}{\bar{\sigma}_j^2} - 1 \right| \left| \log \sigma_j \right|$$

$$\leq \sum_{j=1}^{n} (1 + \epsilon_1^2) \left( \frac{\sigma_1^2}{\bar{\sigma}_j^2} + O \left( \frac{\epsilon_1^2}{\bar{\sigma}_j^2} \right) \right) (2\kappa\epsilon_1 + \kappa^2 \epsilon_1^2) \log \det(A)$$

$$\leq n(\kappa\epsilon_1 + O(\kappa^2 \epsilon_1^2)) + (2\kappa\epsilon_1 + \kappa^2 \epsilon_1^2) \log \det(A)$$

$$= (n + 2) \log \det(A),$$

In the third inequality, we use the result that $\sigma_j \leq \bar{\sigma}_j + \epsilon_1$.

Denote $P'$ as the $\epsilon_2$-approximation of $P$ obtained by amplitude estimation, then the above analysis shows that $-\|A\|^2_2 P' / C^2$ is an $(n + 2) \log \det(A) |(\kappa\epsilon_1 + O(\kappa^2 \epsilon_1^2)) + \kappa^2 \log \kappa) / C^2$ approximation of $\log \det(A)$. Note that

$$\log \det(A) |(\kappa\epsilon_1 + O(\kappa^2 \epsilon_1^2)) + \kappa^2 \log \kappa) = (n + 2n \log \kappa)(\kappa\epsilon_1 + O(\kappa^2 \epsilon_1^2)) + \kappa^2 \log \kappa$$

To make sure the above error is bounded by $\epsilon n$ it suffices to choose $\epsilon_1 = \epsilon / \kappa \log \kappa$ and $\epsilon_2 = \epsilon / \kappa^2 \log \kappa$.

Now we do the runtime analysis. The runtime of the algorithm mainly comes from the using of SVE and the performing of amplitude estimation on the state in (11). By Lemma 25, the complexity to obtain the state (11) is $\tilde{O}(\mu / \epsilon_1)$. The complexity to perform amplitude estimation is $\tilde{O}(\mu \kappa^3 (\log \kappa)^2 / \epsilon^2)$.
B.2 Taylor approximation

As in the classical algorithms, we can first find a polynomial approximation of the logarithm by truncating its Taylor expansion. Then we compute the trace of the polynomial of the matrix. This method has been used in the classical algorithm by Boutsidis et al. [7]. The complexity of their classical algorithm is $\tilde{O}(\|A\|_0 \kappa/\epsilon^2)$. We will show that this algorithm can be quantized with complexity $\tilde{O}(\mu \kappa^2 / \epsilon^2)$. The quantum algorithm has worse dependence on the condition number, but as usual, the dependence on $\|A\|_0$ is relieved, assuming to have quantum access to the matrix $A$. The proof of the following lemma is trivial, and follows from the Taylor expansion of $\log(1-x)$.

**Lemma 36.** Let $A^{n \times n}$ be SPD matrix. Assume that $\|A\| \leq 1$, then

$$\log \det(A) = - \sum_{k=1}^{\infty} \frac{\text{Tr}[(I - A)^k]}{k}.$$  
(12)

The following lemma tells us where to truncate the Taylor series in order to obtain the desired error in the approximation of the log-determinant.

**Lemma 37** (Lemma 8 of [7]). If $m = \lceil \kappa \log(\kappa/\epsilon) \rceil$, then

$$\left| \log \det(A) + \sum_{k=1}^{m} \frac{\text{Tr}[(I - A)^k]}{k} \right| \leq \epsilon |\log \det(A)|.$$  

As for any matrix $B \in \mathbb{R}^{n \times n}$, $\text{Tr}[B] = \sum_{l=1}^{n} |l|B|l|$. So from Lemma 37 we have the quantity that we will estimate with the quantum computer:

$$\log \det(A) \approx -\sum_{k=1}^{m} \frac{\sum_{l=1}^{n} (k)(I - A)^k|l|}{k}.$$  
(13)

**Algorithm 3** Taylor approximation based quantum algorithm for the log-determinant

**Require:** Quantum access to the SPD matrix $A \in \mathbb{R}^{n \times n}$ such that $\|A\| \leq 1, \epsilon \in (0, 1)$, $m = \lceil \kappa \log(1/\epsilon) \rceil$, $B = I - A$, $\epsilon_1 = \epsilon_2 = \epsilon/m$.

**Ensure:** An estimate $|\log \det(A) - \log \det(A)| \leq n \epsilon$.

1: Start from the state $|\psi\rangle = \frac{1}{\sqrt{mn}} \sum_{k=1}^{m} \sum_{l=1}^{n} |k|l|0\rangle$.

2: Apply quantum SVE to precision $\epsilon_1$, followed by a control operation to prepare the state $|\phi\rangle = \frac{1}{\sqrt{mn}} \sum_{k=1}^{m} \sum_{l=1}^{n} |k\left(\sqrt{\frac{B^k}{k}}l|0\rangle + |0\rangle^\perp\right)\rangle$.

3: Apply amplitude estimation to estimate the probability of $|0\rangle$ in $|\phi\rangle$ to precision $\epsilon_2$, denote the result as $L$.

4: Return $\log \det(A) = -mnL$.

**Theorem 38.** Under assumption 34, algorithm 3 returns $\log \det(A)$ such that $|\log \det(A) - \log \det(A)| < \epsilon |\log \det(A)|$ in time $\tilde{O}(\mu \kappa^2 / \epsilon^2)$.

**Proof.** Assume that the SVD of $A$ is $\sum_{j} \sigma_j |u_j\rangle \langle u_j|$. For each $l$, there exist $\beta_1, \ldots, \beta_n$, such that $|l\rangle = \sum_{r} \beta_r |u_r\rangle$. So for the state $|\psi\rangle$, we can rewrite it as

$$|\psi\rangle = \frac{1}{\sqrt{mn}} \sum_{k=1}^{m} \sum_{l=1}^{n} \beta_r |k\rangle |u_r\rangle |0\rangle.$$  

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By Lemma 25, when we perform quantum SVE to this state, we obtain
\[
\frac{1}{\sqrt{mn}} \sum_{k=1}^{m} \sum_{l,r=1}^{n} \beta_{lr} |k⟩|u_r⟩|\tilde{σ}_r⟩,
\]
where |σ_r - \tilde{σ}_r| ≤ \epsilon_1. Apply control rotation to |\tilde{σ}_r⟩, then we obtain
\[
\frac{1}{\sqrt{mn}} \sum_{k=1}^{m} \sum_{l,r=1}^{n} \beta_{lr} |k⟩|u_r⟩ \left( \sqrt{\frac{(1 - \tilde{σ}_r)^k}{k}} |0⟩ + |0⟩^⊥ \right).
\]
Undo the quantum SVE gives rise to the state |φ⟩:
\[
|φ⟩ = \frac{1}{\sqrt{mn}} \sum_{k=1}^{m} \sum_{l,r=1}^{n} \beta_{lr} |k⟩|u_r⟩ \left( \sqrt{\frac{(1 - \tilde{σ}_r)^k}{k}} |0⟩ + |0⟩^⊥ \right) \approx \frac{1}{\sqrt{mn}} \sum_{k=1}^{m} \sum_{l,r=1}^{n} |k⟩ \left( \sqrt{\frac{B^k}{k}} |l⟩|0⟩ + |0⟩^⊥ \right).
\]
From equation (13) we can derive the following approximation:
\[
\frac{- \log \det(A)}{mn} \approx \frac{1}{mn} \sum_{k=1}^{m} \sum_{l,r=1}^{n} \langle l|B^k|l⟩ \frac{k}{k} = \frac{1}{mn} \sum_{k=1}^{m} \sum_{l,r=1}^{n} |β_{lr}|^2 (1 - σ_r)^k \frac{k}{k}.
\]
The right hand side of the above equation is the square of the amplitude of |0⟩ in the state |φ⟩. Due to the error in quantum SVE and amplitude estimation, we have
\[
\left| L + \frac{\log \det(A)}{mn} \right| \leq \left| L - \frac{1}{mn} \sum_{k=1}^{m} \sum_{l,r=1}^{n} β_{lr}^2 (1 - \tilde{σ}_r)^k \frac{k}{k} \right| + \frac{1}{mn} \sum_{k=1}^{m} \sum_{l,r=1}^{n} |β_{lr}|^2 (1 - σ_r)^k \frac{k}{k} \left( 1 - σ_r^k \right)
\]
\[
\leq \epsilon_2 + \frac{1}{mn} \sum_{k=1}^{m} \sum_{l,r=1}^{n} \left| β_{lr}^2 (1 - \tilde{σ}_r)^k \frac{k}{k} \right| + \left| \epsilon \log \det(A) \right| \frac{1}{mn}
\]
\[
\leq \epsilon_2 + \epsilon_2 \frac{1}{mn} \sum_{k=1}^{m} \sum_{l,r=1}^{n} |β_{lr}|^2 + \epsilon \frac{\log \det(A)}{mn}
\]
\[
\leq \epsilon_1 + \epsilon_2 + \epsilon \frac{\log \det(A)}{mn}.
\]
In the second inequality, \epsilon_2 is caused by amplitude estimation, \epsilon \log \det(A)/mn is caused by Taylor expansion (see Lemma 37). So we can choose \epsilon_1 = \epsilon_2 = \epsilon/m. The total cost is thus \(O(\mu/\epsilon_1) = O(\mu \epsilon^{-2} \kappa^2 \log^2(1/\epsilon))\).

**B.3 Chebyshev approximation**

In [29], Han et al. used Chebyshev approximation to estimate the log-determinant of A. This gave a better result than the algorithm based on the Taylor approximation. Again, we assume that \|A\| ≤ 1 and define \(B = I - A\) with \|B\| ≤ 1. By Chebyshev approximation, we have
\[
\log \det A = \text{Tr} \log(I - B) \approx \sum_{j=0}^{d} c_j \text{Tr}[T_j(B)]
\]
where \(T_j(x)\) is the j-th Chebyshev polynomial of first kind, it is defined recursively by \(T_{j+1}(x) = 2xT_j(x) - T_{j-1}(x)\) for \(j \geq 1\), and \(T_0(x) = 1, T_1(x) = x\). In equation (14), \(c_0 = -\log(2), c_j = -2/j\) for \(j \geq 1\).
**Lemma 39** (Theorem 1 and Lemma 7 of [29]). Let \(A \in \mathbb{R}^{n \times n}\) be a positive definite matrix whose eigenvalues are in \([\delta, 1 - \delta]\) for \(\delta \in (0, 1/2]\). Then

\[
\left| \log \det(A) - \sum_{j=0}^{d} c_j \text{Tr}[T_j(I - A)] \right| \leq \frac{20n \log(2/\delta)}{K^{d}(K-1)},
\]

where \(K = \frac{\sqrt{n^2 - n} + \sqrt{n}}{\sqrt{n^2 - n} - \sqrt{n}}\). If we choose \(d = O(\sqrt{\log \epsilon})\), then the error is bounded by \(O(n\epsilon)\).

**Algorithm 4** Chebyshev approximation

**Require:** Quantum access to matrices \(A \in \mathbb{R}^{n \times n}\), \(\epsilon \in (0, 1)\), \(d = \sqrt{n} \log(\kappa / \epsilon)\) and \(\epsilon_1 = \epsilon / \log d\), \(B = I - A\).

**Ensure:** An estimate \(|\log \det(A) - \log \det(A)| \leq n\epsilon\).

1. Set \(c_0 = -\ln(2), c_j = -2/j\). Prepare \(|\phi_1\rangle = \frac{1}{\sqrt{nC}} \sum_{j=0}^{d} \sqrt{-c_j} |j\rangle \otimes \sum_{k=1}^{n} |0\rangle |k\rangle\), \(|\phi_2\rangle = \frac{1}{\sqrt{nC}} \sum_{j=0}^{d} \sqrt{-c_j} |j\rangle \otimes \sum_{k=1}^{n} (|0\rangle T_j(B) |k\rangle + |0\rangle \perp)\).

where \(C = -\sum_{j=0}^{d} c_j\).

2. Apply inner product estimation subroutine between the two states, with precision \(\epsilon_1\). Denote the result as \(P\).

3. Return \(\log \det(A) = -nCP\).

**Lemma 40** (Section 4.3 of [12]). For any quantum state \(|\psi\rangle\), there is a quantum circuit that can implement the mapping

\( |\psi\rangle \mapsto |0\rangle T_j(B) |\psi\rangle + |0\rangle \perp\).

The gate complexity is \(O(j (\log n + \log^{2.5}(\kappa(B)\mu/\epsilon)))\).

**Theorem 41.** Under assumption 34, algorithm 4 returns \(\log \det(A)\) such that \(|\log \det(A) - \log \det(A)| < \epsilon|\log \det(A)|\) in time \(O(\mu \kappa^2 / \epsilon^2)\).

**Proof.** By Lemma 40 each state \(|0\rangle T_j(B) |k\rangle + |0\rangle \perp\) is implemented in time \(O(j (\log n + \log^{2.5}(\kappa(B)\mu/\epsilon)))\). Consequently, \(|\phi_2\rangle\) is prepared in time \(O(d^2 (\log n + \log^{2.5}(\kappa(B)\mu/\epsilon)))\). Note that

\[
C = -\sum_{j=0}^{d} c_j = \log(2) + \sum_{j=1}^{d} \frac{2}{\log(2) + 2(\ln(d) + \frac{1}{2d})} = O(\log d),
\]

\[
\langle \phi_1 | \phi_2 \rangle = -\frac{1}{nC} \sum_{j=0}^{d} \sum_{k=1}^{n} c_j |k\rangle T_j(B) |k\rangle,
\]

\[
\log \det A \approx \sum_{j=0}^{d} \sum_{k=1}^{n} c_j |k\rangle T_j(B) |k\rangle.
\]

About \(C\), we use the fact about the Harmonic number \(H_d = \sum_{j=1}^{d} 1/j\). It is close to \(\frac{1}{2d} + \ln d + \gamma\), where \(\gamma\) is the Euler-Mascheroni constant. Using the test or an inner product estimation procedure, i.e. lemma 33, we obtain an \(\epsilon_1\)-approximation, denoted as \(P\), of \(|\langle \phi_1 | \phi_2 \rangle\). Then

\[
|ncP + \log \det(A)| \leq |nCP + nC|\langle \phi_1 | \phi_2 \rangle| + |nC|\langle \phi_1 | \phi_2 \rangle + \log \det(A)| \leq n(\log d)\epsilon_1 + n\epsilon.
\]

By choosing \(\epsilon_1 = \epsilon / \log d\) leads an error of \(2n\epsilon\). The total cost is \(O(d^2 \epsilon^{-1} (\log d)(\log n + \log^{2.5}(\kappa(B)\mu/\epsilon)))\). Since \(|A| \leq 1\), by considering \(A/2\), without loss of generality, we can assume that \(1/\kappa < \sigma_j < c < 1\) for some constant \(c\), then \(\kappa(B) = (1 - \sigma_{\text{min}})/(1 - \sigma_{\text{max}}) \leq 1/(1-c) = O(1)\). Substitute this into the complexity gives the claimed result. \(\square\)
B.4 Monte Carlo Method

In this section, we present a quantum algorithm that leverage quantum singular value estimation and quantum Monte Carlo methods to estimate the log-determinant. This can be seen as an improvement upon the work of [66], where they used (implicitly) the classical Monte Carlo method, by using a quantum computer to sample from the uniform distribution of singular values of a matrix. In the following, we show how to apply the quantum Monte Carlo method [46] to this problem. This will lead to a better dependence on precision. In their work, they assume to work only with sparse matrices, due to the limitations of previous Hamiltonian simulation techniques. Under the assumption of having quantum access to $A$, their algorithm still works for non-sparse matrices.

**Lemma 42** (Sampling-based algorithm for log-determinant [66]). Under Assumption 34, there is a quantum algorithm that estimates $\log \det(A)$ such that $|\log \det(A) - \log \det(A)| < \epsilon |\log \det(A)|$ in time $O(\mu \kappa / \epsilon^3)$.

While the authors proved in [66] that the variance of the resulting estimator is good enough to be used in the training of Gaussian processes, the variance of this estimator is better analyzed in the following theorem.

**Lemma 43** (Variance of Zhao's estimator). Let $A \in \mathbb{R}^{n \times n}$ such that $\|A\| \leq 1$. Let $\bar{\log \det(A)}$ be the estimate of $\log \det(A)$ using the algorithm described in lemma 42 with error parameter $\epsilon$. Then:

$$\text{Var}(\bar{\log \det(A)}) = \frac{(n \epsilon \log \kappa)^2}{12}.$$  

**Proof.** It is straightforward application of the Bienamé's formula. $\Box$

**Lemma 44.** Let $\sigma_j \in [1/\kappa, 1/2]$. It follows that $\mathbb{E}[\log(1/\bar{\sigma}_j)] \geq 1$, and $\mathbb{E}[\log^2(1/\bar{\sigma}_j)] \leq \log^2 \kappa$. Then:

$$\text{Var}[\log(1/\bar{\sigma}_j)] \leq (\log^2 \kappa - 1) \mathbb{E}[\log(1/\bar{\sigma}_j)]^2.$$  

**Proof.** The proof is straightforward, $\mathbb{E}[\log(1/\bar{\sigma}_j)] = (1/n) \sum_{j=1}^n \log 1/\bar{\sigma}_j \geq 1$. On the other hand, $\mathbb{E}[\log^2(1/\bar{\sigma}_j)] = (1/n) \sum_{j=1}^n \log^2(1/\bar{\sigma}_j) \leq \log^2 \kappa$. So we have

$$\frac{\text{Var}[\log(1/\bar{\sigma}_j)]}{\mathbb{E}[\log(1/\bar{\sigma}_j)]^2} = \frac{\mathbb{E}[\log^2(1/\bar{\sigma}_j)] - \mathbb{E}[\log(1/\bar{\sigma}_j)]^2}{\mathbb{E}[\log^2(1/\bar{\sigma}_j)]^2} \leq \log^2 \kappa - 1.$$  

In this algorithm, we create a state $|\phi_1\rangle$ (defined in equation (16). This state defines a uniform distribution on the singular values $\bar{\sigma}_j$ (or equivalently on $\log(1/\bar{\sigma}_j)$). We apply the quantum Monte Carlo method in order to sample from this state faster. We now recall the quantum Monte Carlo algorithm, result of [46].

**Algorithm 5** Quantum Monte Carlo for the log-determinant

**Require:** Quantum access to the SPD matrix $A \in \mathbb{R}^{n \times n}$, and $\epsilon \in (0, 1)$. Set $\epsilon_1 = \epsilon / \kappa$.

**Ensure:** An estimate $|\log \det(A) - \log \det(A)| \leq n \epsilon$.

1: Prepare

$$|\phi_0\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^n |j, j\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^n |u_j, \bar{u}_j\rangle.$$  

(15)

2: Perform SVE, i.e. Lemma 25 up to precision $\epsilon_1$ to prepare

$$|\phi_1\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^n |u_j, \bar{u}_j\rangle |\bar{\sigma}_j\rangle.$$  

(16)

3: Run algorithm 4 of [46] to estimate $\mathbb{E}[\log(1/\bar{\sigma}_j)]$, set the result as $\tilde{\mathbb{E}}[\log(1/\bar{\sigma}_j)]$.

4: Return $\bar{\log \det(A)} = n \tilde{\mathbb{E}}[\log(1/\bar{\sigma}_j)]$.

**Lemma 45** (Theorem 2.6 of [46]). Assume that there is an Algorithm $A$ that outputs a random variable $v(A)$ after each execution. Denote $|\psi\rangle = A(0), U = 2|\psi\rangle\langle\psi| - I$. If $\text{Var}[v(A)]/\mathbb{E}[v(A)]^2 \leq B$, then, there is a quantum algorithm that uses $O(B)$ copies of $|\psi\rangle$, uses $O(B/\epsilon)$ times of $U$ and outputs $\tilde{\mu}$ such that $\text{Pr}[|\tilde{\mu} - \mathbb{E}[v(A)]| \geq \epsilon \mathbb{E}[v(A)]] \leq 1/4$.  

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We can view \( \mathcal{A} \) as the first two steps of the algorithm 5, that builds a state that is interpreted as a random variable \( \log(1/\tilde{\sigma}_j) \) with probability \( 1/n \). So in step 3, we can use Lemma 45 to estimate \( \mathbb{E}[\log(1/\tilde{\sigma}_j)] \).

**Theorem 46.** Under assumption 34, algorithm 5 returns \( \log \det(A) \) such that \( |\log \det(A) - \log \det(A)| < \epsilon |\log \det(A)| \) in time \( \tilde{O}(\mu\kappa/\epsilon^2) \).

**Proof.** By Lemma 45, in step 3 of Algorithm 5 we can obtain with high probability an estimate \( \log \det(A) := \tilde{\mathbb{E}}[\log(1/\tilde{\sigma}_j)] \) such that:

\[
|\tilde{\mathbb{E}}[\log(1/\tilde{\sigma}_j)] - \mathbb{E}[\log(1/\tilde{\sigma}_j)]| \leq \epsilon \mathbb{E}[\log(1/\tilde{\sigma}_j)].
\]

The cost is \( \tilde{O}(\mu/\epsilon_1 \epsilon) \) due to Lemma 44. Since

\[
|\mathbb{E}[\log(1/\tilde{\sigma}_j)] - \mathbb{E}[\log(1/\sigma_j)]| \leq \frac{1}{n} \sum_{j=1}^{n} |\log \tilde{\sigma}_j - \log \sigma_j| \leq \frac{1}{n} \sum_{j=1}^{n} \frac{\epsilon_1}{\sigma_j} \leq \frac{\epsilon_1}{\sigma_n} = \kappa \epsilon_1,
\]

we can set \( \epsilon_1 = \epsilon/\kappa \) to control the final error is \( (n + \log \det(A))\epsilon \). Thus, we obtain \( \log \det(A) \) in time \( \tilde{O}(\mu\kappa/\epsilon^2) \). \( \square \)