Path Integration on a Quantum Computer*

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Abstract

We study path integration on a quantum computer that performs quantum summation. We assume that the measure of path integration is Gaussian, with the eigenvalues of its covariance operator of order $j^{-k}$ with $k > 1$. For the Wiener measure occurring in many applications we have $k = 2$. We want to compute an $\varepsilon$-approximation to path integrals whose integrands are at least Lipschitz. We prove:

- Path integration on a quantum computer is tractable.
- Path integration on a quantum computer can be solved roughly $\varepsilon^{-1}$ times faster than on a classical computer using randomization, and exponentially faster than on a classical computer with a worst case assurance.
- The number of quantum queries needed to solve path integration is roughly the square root of the number of function values needed on a classical computer using randomization. More precisely, the number of quantum queries is at most $4.22\varepsilon^{-1}$. Furthermore, a lower bound is obtained for the minimal number of quantum queries which shows that this bound cannot be significantly improved.

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• The number of qubits is polynomial in \( \varepsilon^{-1} \). Furthermore, for the Wiener measure the degree is 2 for Lipschitz functions, and the degree is 1 for smoother integrands.

1 Introduction

Although quantum computers currently exist only as prototypes in the laboratory, we believe it is important to study theoretical aspects of quantum computation and to investigate its potential power. There will be additional incentives to try to build quantum computers if it can be shown that there are substantial speed-ups for a variety of problems.

To date there have been two major algorithms for discrete problems on quantum computers that are significantly better than on classical computers: Shor’s factorization and Grover’s data search algorithms, see [4, 5, 19, 20]. But numerous problems in science and engineering have continuous mathematical models. Examples include high dimensional integrals, path integrals, partial differential and integral equations, and continuous optimization.

Continuous problems are usually solved numerically; they can only be solved to within uncertainty \( \varepsilon \). The computational complexity of these problems on classical computers is often known; for a recent survey see [23]. Complexity is defined to be the minimal number of function values and arithmetic operations needed to solve the problem to within \( \varepsilon \).

For many continuous problems defined on functions of \( d \) variables, the complexity in the worst case deterministic setting is exponential in \( \varepsilon^{-1} \) or in \( d \). In the latter case, the problem is said to suffer from the “curse of dimensionality” and is computationally intractable. For some continuous problems the curse of dimensionality can be vanquished by weakening the worst case deterministic assurance to a stochastic assurance, such as in the randomized setting. Monte Carlo is a prime example of an algorithm in the randomized setting.

A start has been made toward solving continuous problems on quantum computers in recent papers [1, 6, 7, 8, 9, 16, 17]. They study multivariate integration and approximation. The major technical tool in these papers is the quantum summation algorithm of Brassard, Hoyer, Mosca and Tapp that is based on Grover’s iterate, see [2, 4]. The essence of the results of Heinrich and Novak, [7, 8, 16], is that intractability in the worst case setting of multivariate integration in a Sobolev space is broken by the use of the quantum summation algorithm. That is, we have an exponential speed-up of quantum algorithms over deterministic algorithms with a worst case assurance. Furthermore, there is roughly a quadratic speed-up of quantum algorithms over randomized algorithms run on a classical computer.

Our paper is a continuation of the idea of using quantum summation for continuous problems. Summation is often required for continuous problems. Algorithms such as Monte Carlo and Quasi-Monte Carlo are used for a variety of continuous problems and they require the summation of many terms. In the worst case setting, the number of terms \( n \) is often an
exponential function of $\varepsilon^{-1}$. However, if we perform summation on a quantum computer, this is not a show stopper, since the cost of the quantum summation algorithm depends only logarithmically on $n$. Hence, as long as $n$ is a single exponential function of $\varepsilon^{-1}$ the quantum cost is polynomial, and the problem becomes tractable on a quantum computer. In this paper we show that quantum summation is a powerful tool for computing also path integrals.

Path integrals may be viewed as integration of functions of infinitely many variables. They occur in many fields, including quantum physics and chemistry, differential equations, and financial mathematics. Efficient algorithms for approximating path integrals are therefore of great interest. However, and perhaps not surprisingly, path integration is intractable on a classical computer in the worst case setting for integrands with finite smoothness as shown in [25]. Fortunately, the worst case complexity of path integration is only a single exponential function in $\varepsilon^{-1}$ if the measure of path integration is Gaussian and the eigenvalues of the covariance operator are of order $j^{-k}$ for $k > 1$. For the Wiener measure, which appears in many applications, we have $k = 2$. That is why when we use the quantum summation algorithm, path integration becomes tractable on a quantum computer. More precisely, for functions having smoothness $r$, see the precise definition of the class $F_r$ in Section 3, path integrals can be computed using of order

- $\varepsilon^{-1}$ quantum queries,
- $\varepsilon^{-(k+\gamma(r))/(k-1)} \log \varepsilon^{-1}$ quantum operations, and
- $\varepsilon^{-(1+\gamma(r))/(k-1)} \log \varepsilon^{-1}$ qubits.

Here $\gamma(1) = 1$ and $\gamma(r) = 0$ for $r \geq 2$. For the Wiener measure, we have more specific bounds, which we present in Theorem 2. We stress that the cost of a quantum query depends on a particular applications and may be very large.

We know more precise bounds on the number of quantum queries. To explain them we comment on two types of errors for path integration. The first error occurs when we replace the original problem by finite dimensional Gaussian integration, and then the second one when we approximate the finite dimensional problem by a finite sum. For simplicity, we assume that the both errors are bounded by $\varepsilon/2$ so that the total error is at most $\varepsilon$. Hence, we need to apply the quantum summation algorithm with error $\varepsilon/2$. To get a $\delta$-error, the quantum summation algorithms requires at most $2.11\delta^{-1}$ quantum queries and this bound is in general sharp, see [11]. Hence, for $\delta = \varepsilon/2$ we need at most $4.22\varepsilon^{-1}$ quantum queries.

Obviously, we may reduce the number of quantum queries by choosing a different splitting of the two errors for path integration. So, if the first error is, say, $a\varepsilon$ and the second is $(1-a)\varepsilon$ for some $a \in (0,1)$, the number of required quantum queries is at most $2.11\varepsilon^{-1}/(1-a)$, and for small $a$ it is roughly at most $2.11\varepsilon^{-1}$. This can be achieved at the expense of increasing quantum operations and qubits.
We also study the question what is the minimal number of quantum queries for solving path integration by an arbitrary quantum algorithm. Similarly as in [16], we show that path integration is no easier than a specific summation problem. Then using the lower bound of [12], we conclude that the minimal number of quantum queries is at least of order $\varepsilon^{-1+\alpha}$ for any $\alpha \in (0,1)$, see Theorem 3. This means that the number of quantum queries used by the algorithm presented in this paper cannot be significantly improved.

We stress that the number of qubits is polynomial in $\varepsilon^{-1}$. Furthermore, for the Wiener measure the degree is 2 for $r = 1$, and 1 for $r \geq 2$. Hence, if $\varepsilon$ is relatively large we do not need too many qubits to solve path integration on a quantum computer. This is important since the number of qubits will be a limiting resource for the foreseeable future.

From these bounds and from the known complexity bounds in the worst case and randomized settings, we conclude that

- Path integration on a quantum computer can be solved roughly $\varepsilon^{-1}$ times faster than on a classical computer using randomization, and exponentially faster than on a classical computer with a worst case assurance.

- The number of quantum queries is the square root of the number of function values needed on a classical computer using randomization.

We outline the remainder of this paper. In Section 2 we briefly discuss the complexity of summation in the worst case and randomized settings, and the quantum summation algorithm for computing the arithmetic mean of $n$ numbers, each from the interval $[-1,1]$. In Section 3 we define path integration precisely, while in Section 4 we explain a computational approach to path integration. In Section 5 we summarize what is known about the complexity of path integration on a classical computer in the worst case and randomized settings. We also outline an algorithm of Curbera, [13], which requires exponentially many function values in the worst case setting, and which is the basis for the quantum path integration algorithm. In Section 6 we discuss path integration on a quantum computer and summarize the advantages of the quantum algorithm. In Section 7 we prove that the upper bound on the number of quantum queries presented in Section 6 is essentially minimal. In the Appendix we present the proof of how many variables must be used to approximate path integrals to within $\varepsilon$.

## 2 Quantum Summation Algorithm

Sums occur frequently in scientific computation. For example, when Monte Carlo or Quasi-Monte Carlo are used to approximate a $d$-dimensional integral, we compute $n^{-1} \sum_{i=1}^{n} f(x_i)$, where the $x_i$ are $d$-dimensional vectors that are chosen randomly (for Monte Carlo) or deterministically (for Quasi-Monte Carlo), see e.g., [13]. As we shall see in Section 5, such
algorithms can be also used for approximating path integrals. In fact, for many linear problems it is known that linear algorithms enjoy many optimality properties, see e.g., \cite{14, 22, 23}. Linear algorithms have the form $\sum_{i=1}^{n} a_i f(x_i)$ for coefficients $a_i$ that are sometimes, but not always, equal to $n^{-1}$. Let $y_i = a_i f(x_i) n$. Then for all these applications we wish to compute

$$S_n(y) = n^{-1} \sum_{i=1}^{n} y_i. \quad (1)$$

In this paper we restrict ourselves to the case when $|y_i| \leq 1$ for $i = 1, 2, \ldots, n$. More general conditions on the $y_i$ of the form $(n^{-1} \sum_{i=1}^{n} |y_i|^p)^{1/p} \leq 1$ with $p \in [1, \infty]$ are considered in \cite{3,4,8,9}.

We are interested in applications where $n$ is huge. We wish to approximate $S_n$ to within $\varepsilon$ for $\varepsilon \in (0, \frac{1}{2})$. The terms $y_i$ are not stored or computed in advance. We assume that for a given index $i$ we have a subroutine that computes $y_i$. This assumption is typical for scientific problems where, as explained above, $y_i$ depends on the function value $f(x_i)$.

Before we discuss quantum computation of $S_n$, we briefly mention summation complexity results in the worst case and randomized settings on a classical computer, see \cite{14,16}. The worst case complexity, $\text{comp}_{\text{wor}}(n, \varepsilon)$, is defined as the minimal number of operations needed to compute an $\varepsilon$-approximation to $S_n$ for all $|y_i| \leq 1$ using deterministic algorithms. The randomized complexity, $\text{comp}_{\text{ran}}(n, \varepsilon)$, is defined analogously when we permit randomized algorithms. It is known that

$$\text{comp}_{\text{wor}}(n, \varepsilon) \approx n (1 - \varepsilon),$$

and if $n \gg \varepsilon^{-2},$

$$\text{comp}_{\text{ran}}(n, \varepsilon) \approx \varepsilon^{-2}.$$  

Hence, in the worst case setting we must add essentially all $n$ numbers, whereas in the randomized setting it is enough to add only $\varepsilon^{-2}$ terms and this, of course, can be achieved by the Monte Carlo algorithm that chooses $\varepsilon^{-2}$ samples from the set $\{y_1, y_2, \ldots, y_n\}$, each with probability $n^{-1}$, and computes their arithmetic mean. This speed-up is significant.

We now turn to what is known about summation on a quantum computer. We wish to compute $QS_n(y, \varepsilon)$ which approximates $S_n(y)$ to within $\varepsilon$ with probability at least $\frac{3}{4}$. That is, $QS_n(y, \varepsilon)$ is a random variable for which the inequality $|S_n(y) - QS_n(y, \varepsilon)| \leq \varepsilon$ holds with probability at least $\frac{3}{4}$. The performance of a quantum algorithm can be summarized by the number of quantum queries, quantum operations and qubits which are used, see \cite{2,5,6,16} for precise definitions of quantum computation and quantum algorithms. Here, we only mention that the quantum algorithm obtains information on the terms $y_i$ by using only quantum queries. The number of quantum operations is defined as the total number of
bit operations performed by the quantum algorithm, and the number of qubits is defined as $k$ if all quantum computations are performed in the Hilbert space of dimension $2^k$.

Since the number of qubits will be a limiting resource for the foreseeable future, it is important to seek algorithms which require as few qubits as possible.

Brassard, Høyer, Mosca and Tapp, see [2], presented a quantum algorithm $QS_n$ that solves the summation problem. Their algorithm is based on Grover’s iterate, see [2, 5], and uses quantum Fourier and Walsh-Hadamard transforms that can be implemented by well known quantum gates. Assume that $n \gg \varepsilon^{-1}$. Then the algorithm $QS_n$ uses of order $\varepsilon^{-1}$ quantum queries,

$\varepsilon^{-1} \log n$ quantum operations,

$\log n$ qubits.

More precise bounds are known about the number of quantum queries. In [11], it is shown that the quantum algorithm $QS_n$ uses at most $\varepsilon^{-1}2.10\ldots$ quantum queries and this bound is sharp for small $\varepsilon$ and large $\varepsilon n$. Due to the lower bound of Nayak and Wu, see [12], the number of quantum queries of any quantum algorithm that solves the summation problem must be at least of order $\varepsilon^{-1}$. Hence, the algorithm $QS_n$ uses almost the minimal number of quantum queries. (In this paper log denotes $\log_2$.)

We can run the quantum algorithm $QS_n$ several times to increase the probability of success. If we want to solve the problem with probability $1 - \delta$, then we should run $QS_n$ roughly $\log \delta^{-1}$ times and take the median as our final result. Then the number of queries and quantum operations is multiplied by $\log \delta^{-1}$, but the number of qubits stays the same.

Of course, these quantum results are of interest only if $\varepsilon^{-1}$ is significantly less than $n$. Fortunately, this is the case for a number of important problems. Indeed, this paper will supply one more such problem, namely, path integration.

So far we assumed that we summed numbers from the interval $[-1, 1]$. The interval $[-1, 1]$ is taken only for simplicity. If we have the interval $[-M, M]$ then we can rescale the summands to $y_i/M$, and multiply the computed result by $M$. This corresponds to the previous problem over the interval $[-1, 1]$ with $\varepsilon/M$. Note, however, that for large $M$, and $n > M/\varepsilon$, the quantum cost is of order $M/\varepsilon$, which is significantly larger than $1/\varepsilon$.

3 Definition of Path Integration

We now define path integrals studied in this paper, see also [25]. Let $X$ be an infinite dimensional separable Banach space equipped with a probability measure $\mu$. We assume that $\mu$ is a zero mean Gaussian measure, see e.g., [24]. The space $X$ can be embedded in the
Hilbert space $H = L_2([0, 1])$ for which the embedding $\text{Im} : X \to H$ is a continuous linear operator. The inner product of $H$ is denoted by $\langle \cdot, \cdot \rangle_H$. Then the measure $\nu = \mu \text{Im}^{-1}$ is also a zero mean Gaussian measure on the Hilbert space $H$. Let $C_\nu$ be the covariance operator of $\nu$, i.e., $C_\nu : H \to H$ and

$$
\langle C_\nu h_1, h_2 \rangle_H = \int_H \langle h_1, h \rangle_H \langle h, h_2 \rangle_H \nu(dh) \quad \forall h_1, h_2 \in H.
$$

The operator $C_\nu$ is self adjoint, nonnegative definite and has a finite trace. We can assume that there exists an orthonormal system $\{\eta_i\}$ from $\text{Im}(X)$, $\langle \eta_i, \eta_j \rangle_H = \delta_{i,j}$, for which

$$
C_\nu \eta_i = \lambda_i \eta_i,
$$

$$
\lambda_1 \geq \lambda_2 \geq \cdots \geq 0 \quad \text{and} \quad \sum_{i=1}^{\infty} \lambda_i < +\infty. \quad (2)
$$

We illustrate this definition by the important example of the space $X = C([0, 1])$ of continuous functions defined on $[0, 1]$ with the sup norm, $\|x\| = \max_{t \in [0, 1]} |x(t)|$. The space $C([0, 1])$ is equipped with the classical Wiener measure $\mu = w$. The measure $w$ is a zero mean Gaussian measure with covariance function $\min(t, u)$. That is,

$$
\int_{C([0,1])} x(t) \, w(dx) = 0 \quad \forall t \in [0, 1],
$$

$$
\int_{C([0,1])} x(t) x(u) \, w(dx) = \min(t, u) \quad \forall t, u \in [0, 1].
$$

For the Wiener measure $w$, we have $\text{Im}(x) = x$ and

$$
\eta_i = \sqrt{2} \sin \left( \frac{2i - 1}{2} \pi x \right), \quad \lambda_i = \frac{4}{\pi^2(2i - 1)^2}.
$$

We return to the case of general $X$ and $\mu$. Let $F$ be a class of real-valued $\mu$-integrable functions defined on $X$. The path integration problem is defined as approximating integrals of $f$ from $F$,

$$
I(f) := \int_X f(x) \mu(dx) = \int_H f(\text{Im}^{-1}x) \nu(dx), \quad \forall f \in F. \quad (3)
$$

If only finitely many eigenvalues $\lambda_i$ of $C_\nu$ are positive, then the measure $\nu$ is concentrated on a finite dimensional subspace of $H$ and path integration reduces to a finite dimensional Gaussian integration. To preserve the main feature of the path integration problem, which is
integration over an infinite dimensional space, we assume that all eigenvalues $\lambda_i$ are positive. The element $x$ from $H$ can be written as $x = \sum_{i=1}^{\infty} t_i \eta_i$, with $t_i = \langle x, \eta_i \rangle_H$. Therefore the integrand $f$ in (3) depends on infinitely many variables $t_i$. That is why the path integration problem can be viewed as integration of functions having infinitely many variables.

In this paper we will consider the classes $F_r$ of functions whose $r - 1$ times Frechet derivatives exist and are bounded, and whose $r$th Frechet derivatives satisfy the Lipschitz condition. More precisely, for a non-negative integer $i$, let $\|f(i)\| = \sup_{x \in X} \|f(i)(x)\|$. Here, $f(i)(x)$ is an $i$-linear form from $X^i$ to $\mathbb{R}$, and its norm is defined as $\|f(i)(x)\| = \sup_{\|x_j\| \leq 1} |f(i)(x)x_1x_2 \cdots x_i|$. Obviously, $\|f(0)\| = \|f\| = \sup_{x \in X} |f(x)|$.

Let $r$ be a positive integer. For positive numbers $K_0,K_1,\ldots,K_r$, define $\|f\|_{r-1} = \max_{0 \leq i \leq r-1} \|f(i)\|/K_i$. The class $F_r$ is defined as

$$F_r = \{ f : \|f\|_{r-1} \leq 1, \|f^{(r-1)}(x) - f^{(r-1)}(y)\| \leq K_r \|\text{Im}(x-y)\|_H, \forall x, y \in X \}.$$ 

For $r = 1$, the class $F_1$ consists of bounded Lipschitz functions. The values of $f$ are bounded by $K_0$, and the Lipschitz constant by $K_1$. For $r \geq 2$, the class $F_r$ consists of bounded smooth functions. All functions from $F_r$ are $r-1$ times Frechet differentiable, their $i$th derivatives are bounded by $K_i$ for $i = 0, 1, \ldots, r-1$, and the $(r-1)$st derivatives satisfy the Lipschitz condition with the constant $K_r$.

Note that for any $f \in F_r$, the path integral $I(f)$ is well defined since $f$ is continuous and bounded. From $|f(x)| \leq K_0$ we have $|I(f)| \leq K_0$. If $K_0$ is large we can use a different estimate on $I(f)$. We have $I(f) = f(0) + I(f - f(0))$ and $|I(f - f(0))| \leq K_1 \int_H \|x\| \nu(dx) \leq K_1 \left(\sum_{j=1}^{\infty} \lambda_j \right)^{1/2}$. Hence, $|I(f)| \leq |f(0)| + K_1 \left(\sum_{j=1}^{\infty} \lambda_j \right)^{1/2}$. This estimate can be better than the previous one for large $K_0$.

As we shall see in the next sections, path integration for the class $F_r$ is intractable in the worst case setting. We stress that for other classes of functions, path integration can be tractable even in the worst case setting. An example is provided for the class of smooth integrands occurring in the Feynman-Kac formula, see [10, 18].

### 4 Computational Approach to Path Integration

We want to approximate $I(f)$ to within $\varepsilon$ for all $f \in F$. The approximate computation of $I(f)$ consists of two steps, see [25]. The first is to approximate the infinite dimensional integration $I$ by a $d$-dimensional integration $I_d$, where $d = d(\varepsilon, F)$ is chosen as the minimal integer for which the error of this approximation is at most, say, $\frac{\varepsilon}{2}$. The second step is to compute an approximation to $I_d$ with error at most $\frac{\varepsilon}{2}$. Clearly, we should expect that $d(\varepsilon, F)$ would go to infinity as $\varepsilon$ goes to zero.
More precisely we proceed as follows. Let \( f_d : \mathbb{R}^d \to \mathbb{R} \) be defined for \( t = [t_1, t_2, \ldots, t_d] \in \mathbb{R}^d \) as
\[
f_d(t) = f \left( \operatorname{Im}^{-1}(t_1 \eta_1 + t_2 \eta_2 + \cdots + t_d \eta_d) \right). \tag{4}
\]
Define
\[
I_d(f) = \frac{1}{(2\pi)^{d/2}} \frac{1}{\sqrt{\lambda_1 \lambda_2 \cdots \lambda_d}} \int_{\mathbb{R}^d} f_d(t) \exp (-t_1^2/(2\lambda_1) - \cdots - t_d^2/(2\lambda_d)) \, dt. \tag{5}
\]
Observe that \( I_d \) is a finite dimensional Gaussian integral with the eigenvalues \( \lambda_i \) as variances. Note that the eigenvalues \( \lambda_i \) tend to zero. Indeed, since \( a = \sum_{i=1}^{\infty} \lambda_i < +\infty \) and \( \lambda_i \) are non-increasing then \( \lambda_i \leq a/i \) for all \( i \). Hence, we have decreasing dependence on the successive variables \( t_i \) in (5). For continuous \( f \), we have
\[
I(f) = \lim_d I_d(f_d).
\]
As outlined above, we want to choose the minimal \( d = d(\varepsilon, F) \) such that \( |I(f) - I_d(f)| \leq \varepsilon/2 \) \( \forall f \in F \), and then to compute an \( \varepsilon/2 \)-approximation to a finite-dimensional integral \( I_d(f_d) \). We now find \( d(\varepsilon, F_r) \) for a family of eigenvalues \( \lambda_j \) of the covariance operator \( C_\nu \). The family includes the eigenvalues of \( C_\nu \) for the Wiener measure.

**Theorem 1** Suppose \( \lambda_j \) is of order \( j^{-k} \) with \( k > 1 \). Then
\[
\underline{c}_1 \varepsilon^{-2/(k-1)} \leq d(\varepsilon, F_1) \leq \overline{c}_1 \varepsilon^{-2/(k-1)},
\]
\[
\underline{c}_r \varepsilon^{-1/(k-1)} \leq d(\varepsilon, F_r) \leq \overline{c}_r \varepsilon^{-1/(k-1)} \quad \text{for } r \geq 2,
\]
where \( \underline{c}_r \) and \( \overline{c}_r \), for \( r = 1, 2, \ldots \), are positive numbers independent of \( \varepsilon \) and depending only on the global parameters \( K_i, r, k \) and the trace \( \sum_{i=1}^{\infty} \lambda_i \). In particular, if \( \lambda_j = a j^{-k} \) with \( a > 0 \) then
\[
d(\varepsilon, F_1) \leq 1 + \left( \frac{4aK_1^2}{k-1} \right)^{1/(k-1)} \left( \frac{1}{\varepsilon} \right)^{2/(k-1)},
\]
\[
d(\varepsilon, F_r) \leq 1 + \left( \frac{aK_2}{k-1} \right)^{1/(k-1)} \left( \frac{1}{\varepsilon} \right)^{1/(k-1)} \quad \text{for } r \geq 2.
\]
For the Wiener measure, \( \lambda_j = 4/(\pi^2(2i-1)^2) \), we have
\[
d(\varepsilon, F_1) \leq \left[ \left( \frac{1}{\pi^2} \frac{2K_1}{\varepsilon} \right)^2 + \frac{1}{2} \right],
\]
\[
d(\varepsilon, F_r) \leq \left[ \frac{K_2}{\pi^2 \varepsilon} + \frac{1}{2} \right] \quad \text{for } r \geq 2.
\]
The proof of this theorem is given in the Appendix. We stress that the upper bounds on \( d(\varepsilon, F_r) \) in Theorem 1 depend only on \( K_1 \) for \( r = 1 \), and on \( K_2 \) for \( r \geq 2 \), i.e., on the Lipschitz constants for \( f \) or \( f' \), respectively. This means that we can even take all the remaining \( K_i = \infty \) and the upper bounds on \( d(\varepsilon, F_r) \) still hold. On the other hand, the lower bounds depend on all of the \( K_i \). The dependence is weak since they only affect the multiplicative factors of the power of \( \varepsilon^{-1} \), and the power of \( \varepsilon^{-1} \) does not depend on \( K_i \).

5 Path Integration on a Classical Computer

In this section we discuss approximation of path integrals on a classical computer. We assume the real number model of computation, which is usually used for the analysis of scientific computing problems, see [21] for the rationale. We assume, in particular, that we can perform arithmetic operations (addition, subtraction, multiplication, division), and comparisons of real numbers. We assume that these operations are performed exactly and each costs unity. To approximate path integrals we must have information concerning the integrands \( f \in F \). This information may be supplied by function values \( f(x_i) \) for some \( x_1, x_2, \ldots, x_n \), where \( n = n(\varepsilon, F) \) will be chosen depending on the error demand \( \varepsilon \) and the class \( F \). As outlined in the previous section, we will need to know \( f(x) \) for \( x \) belonging to a finite dimensional subspace \( X_d = \text{span}(\text{Im}^{-1} \eta_1, \text{Im}^{-1} \eta_2, \ldots, \text{Im}^{-1} \eta_d) \) with \( d = d(\varepsilon, F) \).

We therefore assume that we can compute values of \( f(x) \) for \( x \in X_d \) and the cost of one such evaluation is \( c_d \). Usually \( c_d \gg 1 \). Furthermore, we will sometimes assume that the cost \( c_d \) depends linearly on \( d \), i.e., \( c_d = c d \); however, this assumption is not essential to the analysis. For a more complete discussion of the real number model of computation with function values, see [15, 22].

Let \( A(f) \) be any algorithm for approximation of path integrals. The algorithm \( A \) uses a finite number \( n_1 \) of function values at points \( x_i \) and a finite number \( n_2 \) of arithmetic operations and comparisons to compute \( A(f) \). The cost of computing \( A(f) \) is \( c d n_1 + n_2 \). In the worst case setting, the error and cost of \( A \) are defined by its worst performance over the class \( F \). In the randomized setting, the algorithm \( A \) may use randomly chosen samples \( x_i \), and its error and cost are defined by the expected error with respect to the distribution generating the random samples for a worst \( f \) from \( F \). By the worst case or randomized complexity, we mean the minimal cost that is needed to compute an \( \varepsilon \)-approximation for all \( f \in F \), see [22] for precise definitions.

We now briefly discuss the worst case and randomized complexities of path integration for the classes \( F_r \). We begin with the worst case setting. We first state the result of Bakhvalov, see e.g., [14, 22], which states that the worst case complexity of multivariate integration over the unit cube \([0, 1]^d\) for \( r \)-times differentiable functions is of order \( c_d \varepsilon^{-d/r} \).
For path integration $d$ is an increasing function of $\varepsilon^{-1}$, and as shown in Theorem 1, it goes to infinity polynomially in $\varepsilon^{-1}$ as $\varepsilon$ goes zero. This suggest that the worst case complexity, $\text{comp}^{\text{wor}}(\varepsilon, F_r)$, of path integration in the class $F_r$ is exponential in $\varepsilon^{-1}$. A formal proof may be found in [25] for any $r$, and more precise complexity bounds in [3] for $r = 1$. Thus path integration is intractable for the class $F_r$ in the worst case setting. This means that the cost of any algorithm for solving this problem must be exponential. Yet, as we shall see, such algorithms will be useful for quantum computation. We now sketch such an algorithm.

We first consider the case $r = 1$ and then show that an easy modification of the same algorithm can be also used for $r \geq 2$. We assume that $\lambda_j = \Theta(j^{-k})$. From Theorem 1 we know that it is enough to compute an $\varepsilon^{2}$-approximation to the integral $I_d(f)$ with $d = d(\varepsilon, F_1)$ given in Theorem 1. We have

$$I_d(f) = \int_{\mathbb{R}^d} f_d(t) \nu_d(dt),$$

where $\nu_d$ is a Gaussian measure on $\mathbb{R}^d$ with mean zero and with the diagonal covariance matrix $\text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$.

This problem has been studied in [3]. Based on that paper we describe an algorithm $S_n$ with worst case error at most $\varepsilon^{2}$. We opt here for simplicity of the presentation of $S_n$ at a slight expense of its cost. Let $n = m^d$ for the minimal odd integer $m$ for which

$$m \geq \frac{4 K_1 \left( \pi \sum_{i=1}^{d} \lambda_i \right)^{1/2}}{\varepsilon}.$$  

(7)

For $x \geq 0$, let $\psi(x) = \sqrt{2/\pi} \int_0^x \exp(-t^2/2)dt$ be the probability integral, and let $\psi^{-1}$ be its inverse. We note that it is easy to compute $\psi^{-1}(t)$ numerically for any $t \in \mathbb{R}$. As in Lemma 1 of [3], for $i = 1, 2, \ldots, d$ define the points $t_{i,j}$:

$$t_{i,0} = -\infty,$$

$$t_{i,j} = (3\lambda_i)^{1/2} \psi^{-1}((j - 1/2)/m), \quad j = 1, 2, \ldots, m,$$

$$t_{i,m+1} = \infty.$$

Then take $t_{i,j}^* = t_{i,j}$ if $|t_{i,j}| \leq |t_{i,j+1}|$, and $t_{i,j}^* = t_{i,j+1}$ otherwise. For the integer vector $\vec{j} = [j_1, j_2, \ldots, j_d]$, with $j_i = 1, 2, \ldots, m$, define the sample points

$$x_{\vec{j}} = [t_{1,j_1}^*, t_{2,j_2}^*, \ldots, t_{d,j_d}^*].$$

1 We follow a convention of complexity theory that if the complexity growth is faster than polynomial then we say it is exponential.

2 The theta notation means that there exist positive numbers $c_1$ and $c_2$ such that $c_1 j^{-k} \leq \lambda_j \leq c_2 j^{-k}$ for all $j = 1, 2, \ldots$. 11
Then the algorithm takes the simple form

\[ S_n(f_d) = n^{-1} \sum_j f(x_j). \] (8)

Curbera proved in [3] that the worst case error of \( S_n \) is at most

\[ e_{\text{wor}}(S_n) \leq 2K_1 \left( \pi \sum_{i=1}^{d} \lambda_i \right)^{1/2} m^{-1} \leq \frac{\varepsilon}{2}, \]

where the last inequality holds due to the choice of \( m \).

The cost of \( S_n \) is \((c_d + 1)n\) where

\[ n = n(\varepsilon^{-1}) = m^d \leq \left( \frac{\alpha}{\varepsilon} \right)^{\frac{1}{2}d^{-2/(k-1)}}, \] (9)

where \( \alpha = 4K_1 (\pi \sum_{i=1}^{\infty} \lambda_i)^{1/2} + 2\varepsilon \), and \( \pi \) is from Theorem 1.

We now consider the case \( r \geq 2 \). As shown in Theorem 1, we can now restrict ourselves to the integrals \( I_d(f) \) for \( d = d(\varepsilon, F_r) \). We stress that \( d(\varepsilon, F_r) \) is much less than \( d(\varepsilon, F_1) \) for small \( \varepsilon \). Observe that all functions \( f \) from \( F_r \) also belong to \( F_1 \) since they satisfy the Lipschitz condition with the constant \( K_1 \). Hence we can use the algorithm \( S_n \) with the important difference that now \( d = d(\varepsilon, F_r) \). Hence, we compute an \( \frac{\varepsilon}{2} \)-approximation by the algorithm \( S_n \) with cost \((c_d + 1)n\), where

\[ n = n(\varepsilon^{-1}) = m^{d(\varepsilon, F_r)} \leq \left( \frac{\alpha}{\varepsilon} \right)^{\frac{1}{2}d^{-1/(k-1)}}, \] (10)

with \( \frac{\varepsilon}{2} \) from Theorem 1.

We now justify why it is enough to apply the algorithm \( S_n \) for the class \( F_r \) for any \( r \geq 2 \). The reason is that for path integration the smoothness parameter \( r \) is not as important as for finite dimensional integration. Indeed, since the exponent of \( \varepsilon^{-1} \) for the worst case complexity of path integration is unbounded (as \( \varepsilon \to 0 \)) for any fixed \( r \), it does not help much to divide by \( r \).

As we shall see in the next section, for quantum computation the logarithm of the worst case complexity is important and \( r \) can only effect a multiplicative factor. The most important property is how fast \( d(\varepsilon, F_r) \) goes to infinity. As we know from Theorem 1, the influence of \( r \) is significant here since we have different formulas for \( d(\varepsilon, F_r) \) for \( r = 1 \) and \( r \geq 2 \). However, for \( r \geq 2 \), the use of more efficient algorithms than \( S_n \) can only improve the multiplicative factor of the logarithm of the worst case complexity.
We turn to the randomized setting for \( \lambda = \Theta(j^{-k}) \). The randomized complexity, \( \text{comp}_{\text{ran}}(\varepsilon, F_r) \), can be easily obtained by applying results of Bakhvalov for finite dimensional integration. The analysis in [23] yields

\[
\text{comp}_{\text{ran}}(\varepsilon, F_r) = \Theta\left((c_d + 1) \varepsilon^{-2(1+o(1))}\right) \quad \text{as} \quad \varepsilon \to 0, \tag{11}
\]

where \( d = d(\varepsilon, F_r) \) and the factors in the \( \Theta \) notation depend at most quadratically on \( K_0 \) and \( K_1 \). Hence, in the randomized setting we have roughly quadratic dependence in \( \varepsilon^{-1} \) on the number of function values. If \( c_d = c \) then

\[
\text{comp}_{\text{ran}}(\varepsilon, F_r) = \Theta\left(c \left( \frac{1}{\varepsilon} \right)^{1+\gamma(r)k^{-1} + 2 + o(1)} \right) \tag{12}
\]

where \( \gamma(1) = 1 \) and \( \gamma(r) = 0 \) for \( r \geq 2 \).

Hence, the randomized complexity of path integration depends polynomially on \( \varepsilon^{-1} \), and therefore the path integration problem is tractable in the randomized setting. In fact, the upper bound can be achieved by the Monte Carlo algorithm with randomized error at most \( \frac{\varepsilon}{2} \) and with the cost proportional to \( c_d K_0^2 \varepsilon^{-2} \) randomized evaluations of a function of \( d = d(\varepsilon, F_r) \) variables, where \( d(\varepsilon, F_r) \) is given by Theorem 1.

Note, however, that if \( k \) goes to one then the degree of \( \varepsilon^{-1} \) in the randomized complexity goes to infinity. The reason is that in this case we have to compute function values of very many variables. On the other hand, for the Wiener measure we have \( k = 2 \), and the degree of \( \varepsilon^{-1} \) is roughly \( 3 + \gamma(r) \).

6 Path Integration on a Quantum Computer

We now analyze path integration on a quantum computer. The idea behind solving path integration on a quantum computer is quite simple. (However, the analysis is not so simple.) We will apply analogous techniques for other problems in future papers.

Start with an algorithm that computes an \( \varepsilon \)-approximation to path integration in the worst case setting and that requires summation of the form of (11). We run this algorithm on a quantum computer using the quantum summation algorithm of Section 2. Obviously, \( n \) is now a function of \( \varepsilon^{-1} \). For path integration for the class \( F_r \) we know that \( n \) is an exponential function of \( \varepsilon^{-1} \) and is bounded by (11) for \( r = 1 \), and by (10) for \( r \geq 2 \). However, the exponential dependence on \( \varepsilon^{-1} \) is now not so essential since the cost of the quantum summation algorithm \( QS_n \) depends only logarithmically on \( n \). Since \( \log n \) is a polynomial in \( \varepsilon^{-1} \) we conclude that path integration on a quantum computer can be solved at cost
polynomial in \( \varepsilon^{-1} \). That is, intractability of path integration in the worst case setting is broken on a quantum computer by the use of the quantum summation algorithm.

For other intractable problems in the worst case setting for which the worst case complexity can be achieved by summation of \( n \) numbers, intractability will be broken as long as \( n \) is a single exponential function of \( \varepsilon^{-1} \), i.e., \( n(\varepsilon^{-1}) \leq 2^p(\varepsilon^{-1}) \) with \( p \) being a polynomial. Then the quantum cost will be polynomial in \( \varepsilon^{-1} \), and the problem will be tractable on a quantum computer. This idea will not work if \( n(\varepsilon^{-1}) \) is a double exponential function (or worse) of \( \varepsilon^{-1} \) since then the logarithm of \( n(\varepsilon^{-1}) \) will be still an exponential function of \( \varepsilon^{-1} \).

We now provide details of this idea for path integration for the class \( F_r \) with eigenvalues \( \lambda_j = \Theta(j^{-k}) \). We take the algorithm \( S_n \) defined by (8) with \( n \) given by (9) for \( r = 1 \) and by (10) for \( r \geq 2 \). The algorithm \( S_n \) already has the form (4) required by the summation algorithm. However, the summands \( f(x_j) \) are not necessarily in the interval \([-1, 1]\). The function \( f \) belongs to \( F_r \) and therefore its values are bounded by \( K_0 \). Hence, it is enough to scale the problem by running the quantum summation algorithm for \( y_j = f(x_j)/K_0 \), replace \( \varepsilon \) by \( \varepsilon/K_0 \), and multiply the computed result by \( K_0 \). The cost of an algorithm on a quantum computer using \( m \) qubits is defined as on a classical computer with the cost of a quantum query taken as \( c_d \) since \( f(x_j)'s \) are computed and \( m \) qubits are processed by a quantum query. Using the results of quantum summation from Section 2 applied for \( S_n \) we obtain the following theorem.

**Theorem 2** Consider path integration for the class \( F_r \) with the eigenvalues \( \lambda_j = \Theta(j^{-k}) \). Using the quantum summation algorithm \( QS_n \) to compute an \( \varepsilon/K_0 \)-approximation to \( S_n \), we compute an \( \varepsilon \)-approximation for path integrals with probability at least \( \frac{3}{4} \) and of order

\[
\varepsilon^{-((k+\gamma(r))/(k-1))} \log \varepsilon^{-1} \quad \text{quantum operations},
\]

\[
\varepsilon^{-((1+\gamma(r))/(k-1))} \log \varepsilon^{-1} \quad \text{qubits},
\]

where \( \gamma(1) = 1 \) and \( \gamma(r) = 0 \) for \( r \geq 2 \). If \( c_d = c_d \), then the cost of this algorithm is of order

\[
\left( \frac{1}{\varepsilon} \right)^{\frac{1+\gamma(r)}{k-1}+1} \left( c + \log \frac{1}{\varepsilon} \right).
\]

For the Wiener measure the results are more precise. The algorithm requires (neglecting ceilings for simplicity) at most

\[
\frac{2K_0}{\varepsilon} d^{\text{up}}(\varepsilon, F_r) \log \frac{2K_0 \varepsilon^{-1}}{16 K_0 K_1} \quad \text{quantum queries},
\]

\[
\frac{16 K_0 K_1}{\varepsilon} \quad \text{quantum operations},
\]

\[
d^{\text{up}}(\varepsilon, F_r) \log \frac{16 K_0 K_1}{\varepsilon} \quad \text{qubits}.
\]
If $c_d = c_d$, then the cost of this algorithm is at most

$$\frac{2K_0 d^\text{up}(\varepsilon, F_r)}{\varepsilon} \left( c + 2 \log \frac{16 K_0 K_1}{\varepsilon} \right).$$

Here $d^\text{up}(\varepsilon, F_r)$ is an upper bound on $d(\varepsilon, F_r)$ given by

$$d^\text{up}(\varepsilon, F_r) = \left\lceil \left( \frac{K_0 \beta(r)}{\pi^2 \varepsilon} \right)^{1+\gamma(r)} + \frac{1}{2} \right\rceil$$

with $\beta(r) = 2K_1$ for $r = 1$, and $\beta(r) = K_2$ for $r \geq 2$.

If we want to increase the probability of computing an $\varepsilon$-approximation to path integration then, as explained in Section 2, we can run the quantum algorithm for $QS_n$ roughly $\log \delta^{-1}$ times and take the median as the final result. Then the probability of success is at least $1 - \delta$. Obviously the cost is then multiplied by $\log \delta^{-1}$ but the number of qubits stays the same.

We compare $\text{cost}(QS_n)$, the cost of the quantum algorithm, with the worst case complexity of path integration. The essence of Theorem 2 is that $\text{cost}(QS_n)$ depends polynomially on $\varepsilon^{-1}$. Since the worst case complexity is exponential in $\varepsilon^{-1}$, the use of quantum summation breaks intractability of the worst case setting. Note that we have exponential speed-up, i.e., $\text{comp}^{\text{wor}}(\varepsilon, F_r)/\text{cost}(QS_n)$ is exponential in $\varepsilon^{-1}$.

We now compare $\text{cost}(QS_n)$ with the randomized complexity of path integration. As discussed in Section 5, path integration is tractable in the randomized setting and its randomized complexity is characterized by (11) and (12). Comparing the formulas for the randomized complexity with $\text{cost}(QS_n)$ we see that the ratio of the number of quantum queries used by the quantum algorithms to the number of function values used by the best randomized algorithm is roughly $\varepsilon^{-1}$. If we compare $\text{cost}(QS_n)$ to the randomized complexity we see that the speed-up is roughly of order $\varepsilon^{-1}$. That is, we solve path integration on a quantum computer roughly $\varepsilon^{-1}$ times cheaper than on a classical computer using randomization. We summarize our results in the following corollary.

**Corollary 1** Consider path integration for the class $F_r$ with $\lambda_j = \Theta(j^{-k})$. Then

- Path integration on a quantum computer is tractable.

- Path integration on a quantum computer can be solved roughly $\varepsilon^{-1}$ times faster than on a classical computer using randomization, and exponentially faster than on a classical computer with a worst case assurance.
• The number of quantum queries is the square root of the number of function values needed on a classical computer using randomization.

• The number of qubits is polynomial in $\varepsilon^{-1}$. Furthermore, for the Wiener measure the degree is 2 for $r = 1$, and 1 for $r \geq 2$.

7 Lower Bounds on the Number of Quantum Queries

We now study lower bounds on the minimal number $qq(\varepsilon, F_r)$ of quantum queries needed to compute an $\varepsilon$-approximation with probability $3/4$ for path integration for the class $F_r$. From Theorem 2 we know that $qq(\varepsilon, F_r)$ is at most of order $\varepsilon^{-1}$. We show that this bound cannot be significantly improved.

**Theorem 3** Consider path integration for the class $F_r$ with all positive eigenvalues $\lambda_i$. Then

$$\lim_{\varepsilon \to 0} \varepsilon^{1-\alpha} qq(\varepsilon, F_r) = \infty \quad \forall \alpha \in (0, 1).$$

*Proof:* The proof consists of two steps. The first one is to reduce path integration to a finite dimensional Gaussian integration which is no harder than the original problem. The second step is essentially the same as in Novak’s papers, see [14, 16], and reduces the finite dimensional Gaussian integration problem to summation for which the lower bound of Nayak and Wu, see [12], applies.

In the first step of the proof, for a given $\alpha \in (0, 1)$ we take an integer $d > r(1 - \alpha)/\alpha$. (Hence, $d$ is large for small $\alpha$.) The path integration problem for the class $F_r$ is no harder if we assume some additional properties of functions $f$ from $F_r$. We have, see (3),

$$I(f) = \int_H f(\text{Im}^{-1}x) \nu(dx)$$

where $x = \sum_{i=1}^{\infty} t_i \eta_i$.

Let us now assume that $f$ depends only on the first $d$ components $t_1, t_2, \ldots, t_d$, and call this class $F_{r,d}$. Obviously, $F_{r,d}$ is a subclass of $F_r$ and therefore path integration for $F_{r,d}$ is no harder than for the class $F_r$. For the class $F_{r,d}$, the path integration problem reduces to a finite dimensional Gaussian integration problem. That is, for $f \in F_{r,d}$ we have

$$I_d(f) = \int_{\mathbb{R}^d} f_d(t) \nu_d(dt),$$

where $\nu_d$ is the Gaussian measure given by (3), and $f_d$ is given by (4).
The functions \( f_d \) from \( F_{r,d} \) are \( r - 1 \) times continuously differentiable and
\[
\|f_d\| = \sup_{t \in \mathbb{R}^d} |f_d(t)| \leq K_0.
\]
Furthermore, their \( r - 1 \) partial derivatives satisfy the Lipschitz condition. More precisely, there exists a positive number \( \beta_1 \) depending only on \( d, r \) and \( K_0, K_1, \ldots, K_r \) such that
\[
|D^i f_d(t) - D^i f_d(y)| \leq \beta_1 \|t - y\|_\infty \quad \forall t, y \in \mathbb{R}^d,
\]
where \( D^i \) runs through the set of all partial derivatives of order \( r - 1 \).

This shows that the class \( F_{r,d} \) is closely related to the class \( F_{r-1,1}^r \) studied by Novak, see [16],
\[
F_{r-1,1}^r = \{ f : [0, 1]^d \to \mathbb{R} | f \in C^{r-1}([0, 1]^d), |D^i f(t) - D^i f(y)| \leq \|t - y\|_\infty \forall t, y \}\.
\]
Obviously, the different Lipschitz constants: \( \beta_1 \) in our case and 1 for the class \( F_{r-1,1}^r \) do not play a major role since they do not change the order of error bounds. One difference between the two classes is that the common domain of functions from \( F_{r,d} \) is \( \mathbb{R}^d \), whereas for the class \( F_{r-1,1}^r \) the common domain is \([0, 1]^d\). A second difference is that we have Gaussian integration whereas Novak considered uniform integration, \( \int_{[0,1]^d} f(t) dt \). As we shall see below these two differences are not really essential.

In the second step of the proof, we use Novak’s proof technique. From [14, 16] we know that for any positive \( \varepsilon_1 \) there are functions \( f_1, f_2, \ldots, f_n \), with \( n = \Theta(\varepsilon_1^{-d/r}) \), from the class \( F_{r-1,1}^r \) such that they take non-negative values, have disjoint supports in \([0, 1]^d\) and
\[
\begin{align*}
\bullet & \int_{[0,1]^d} f_i(t) dt = \varepsilon_1^{1+d/r} \quad i = 1, 2, \ldots, n, \\
\bullet & \sum_{i=1}^n \alpha_i f_i \in F_{r-1,1}^r \quad \forall |\alpha_i| \leq 1.
\end{align*}
\]
We use the same functions \( f_i \) for our Gaussian integration for the class \( F_{r,d} \). Since the support of \( f_i \) is in \([0, 1]^d\) we can extend \( f_i \) by zero to \( \mathbb{R}^d \). The extended functions \( f_i \) have exactly the same smoothness as required for the class \( F_{r,d} \), and there exists a positive \( \beta_2 \) depending only on \( d, r \) and \( K_0, K_1, \ldots, K_r \) but independent of \( i \) such that \( \beta_2 f_i \in F_{r,d} \). Note that
\[
\int_{\mathbb{R}^d} f_i(t) \nu_d(dt) = \int_{[0,1]^d} \rho_d(t) f_i(t) dt,
\]
where
\[
\rho_d(t) = \frac{1}{\prod_{j=1}^d (2\pi \lambda_j)^{1/2}} \exp \left( -\sum_{j=1}^d t_j^2 / 2 \right).
\]
Since all \( \lambda_j \) are positive, the function \( \rho_d \) has positive minimum and maximum over \([0, 1]^d\). That is, there are positive \( \beta_3 \) and \( \beta_4 \) depending on \( d \) and \( \lambda_1, \lambda_2, \ldots, \lambda_d \) such that

\[
\beta_3 \leq \rho_d(t) \leq \beta_4 \quad \forall t_j \in [0, 1].
\]

Therefore for the functions \( g_i = \beta_2 f_i \in F_{r,d} \) we have

\[
\beta_2 \beta_3 \varepsilon^{1+d/r} \leq I(g_i) = \int_{\mathbb{R}^d} g_i(t) \nu_d(dt) \leq \beta_2 \beta_4 \varepsilon_1^{1+d/r},
\]

and

\[
\sum_{i=1}^n \alpha_i g_i \in F_{r,d} \quad \forall |\alpha_i| \leq 1.
\]

Since

\[
I \left( \sum_{i=1}^n \alpha_i g_i \right) = \sum_{i=1}^n \alpha_i I(g_i)
\]

we reduce our problem to summation of \( n = \Theta(\varepsilon_1^{-d/r}) \) terms for arbitrary \(|\alpha_i| \leq 1\). Let

\[
y_i = \frac{I(g_i)}{\beta_2 \beta_4 \varepsilon_1^{1+d/r}} \alpha_i.
\]

Observe that by varying \( \alpha_i \) from \([-1, 1]\), the \( y_i \) can take any value from \( \beta_3 / \beta_4 [-1, 1] \) due to the left hand side of (13).

We need to compute an \( \varepsilon \)-approximation to \( I(\sum_{i=1}^n \alpha_i g_i) \). This is equivalent to computing an \( \varepsilon_2 \)-approximation to

\[
\frac{1}{n} \sum_{i=1}^n y_i
\]

with \( \varepsilon_2 = \varepsilon / (n \beta_2 \beta_4 \varepsilon_1^{1+d/r}) = \Theta(\varepsilon / \varepsilon_1) \).

The summation problem \( n^{-1} \sum_{i=1}^n y_i \) for our \( y_i \) is not easier than the summation problem \( n^{-1} \sum_{i=1}^n y_i \) for all \(|y_i| \leq \beta_3 / \beta_4 \). We can now apply the lower bound of Nayak and Wu, see [12], that states that the minimal number of quantum queries needed to compute an \( \varepsilon_2 \)-approximation with probability 3/4 for the summation problem \( n^{-1} \sum_{i=1}^n y_i \) with \(|y_i| \leq \beta_3 / \beta_4 \) is bounded from below by

\[
C \min \left( n, \frac{\beta_4}{\beta_3 \varepsilon_2} \right) = \Theta \left( \min(\varepsilon_1^{-d/r}, \varepsilon_1 / \varepsilon) \right),
\]

with some absolute positive number \( C \).
Finally, we take $\varepsilon_1$ such that $\varepsilon_1^{-d/r} = \varepsilon_1/\varepsilon$, i.e., $\varepsilon_1 = \varepsilon^{r/(d+r)}$, and conclude that the minimal number $\text{qq}(\varepsilon, F_r)$ of quantum queries is at least of order $\varepsilon^{-(1-r/(d+r))}$. Since $d > r(1-\alpha)/\alpha$ implies that $\alpha > r/(d+r)$, we have

$$
\varepsilon^{1-\alpha} \text{qq}(\varepsilon, F_r) = \Omega \left( \varepsilon^{-(\alpha-r/(d+r))} \right) \to \infty \quad \text{as} \quad \varepsilon \to 0.
$$

This completes the proof.

8 Appendix

We prove Theorem 1. We begin with $r = 1$. It is shown in [25] that $d = d(\varepsilon, F_1) \leq d^*$ where $d^*$ is an integer satisfying

$$
\sum_{i=d^*+1}^{\infty} \lambda_i \leq \varepsilon^2/(2K_1)^2.
$$

For $\lambda_i = \Theta(i^{-k})$ with $k > 1$, we get

$$
d^* = \Theta \left( (K_1/\varepsilon)^{2/(k-1)} \right) \quad \text{as} \quad \varepsilon \to 0.
$$

For $\lambda_i = ai^{-k}$, we get

$$
d^* = \left\lceil \left( \frac{a}{k-1} \right)^{1/(k-1)} \left( \frac{2K_1}{\varepsilon} \right)^{2/(k-1)} \right\rceil.
$$

For the Wiener measure we have

$$
d^* = \left\lceil \left( \frac{1}{\pi^2 \varepsilon} \right)^2 + \frac{1}{2} \right\rceil.
$$

This establishes upper bounds on $d(\varepsilon, F_1)$.

To get a lower bound, take the function $g : \mathbb{R} \to \mathbb{R}$ defined by $g(x) = c_1|x|/(1 + |x|)$ with $c_1 = \min(K_0, K_1)$. We have $\sup_{x \in \mathbb{R}} |g(x)| = c_1 \leq K_0$, and $g$ satisfies the Lipschitz condition with the constant $c_1 \leq K_1$. For $x \in H$, define $x_d = \sum_{j=d+1}^{2d} \langle x, \eta_j \rangle_H \eta_j$ and

$$
f \left( \text{Im}^{-1} x \right) = g(\|x_d\|).
$$

Then $f \in F_1$ and $f_d = 0$. We have $I(f) - I(f_d) = I(f)$ and

$$
I(f) = \int_H g(\|x_d\|) \nu(dx) \geq c_1 \int_{\|x_d\| \leq 1} \frac{\|x_d\|}{1 + \|x_d\|} \nu(dx) \geq \frac{c_1}{2} \int_{\|x_d\| \leq 1} \|x_d\| \nu(dx).
$$
Since \( \left( \sum_{j=d+1}^{2d} a_j^2 \right)^{1/2} \geq d^{-1/2} \sum_{j=d+1}^{2d} |a_j| \) for any \( a_j \in \mathbb{R} \), we get

\[
I(f) \geq \frac{c_1}{2d^{1/2}} \sum_{j=d+1}^{2d} \text{Int}_j
\]

where

\[
\text{Int}_j = \prod_{i=1}^{d} (2\pi \lambda_i)^{-1/2} \int_{\sum_{i=d+1}^{2d} x_i^2 \leq 1} |x_j| \exp \left( - \sum_{i=d+1}^{2d} x_i^2 / (2\lambda_i) \right) dx.
\]

There exist two positive numbers \( \alpha_1 \) and \( \alpha_2 \) such that \( \alpha_1 i^{-k} \leq \lambda_i \leq \alpha_2 i^{-k} \) for all \( i \). By changing variables \( t_{i-d} = x_i / (\lambda_i)^{1/2} \) and noting that \( \alpha_2 d^{-k} \geq \lambda_d \geq \lambda_i \geq \lambda_2 d \geq \alpha_1 (2d)^{-k} \) we conclude that

\[
\text{Int}_j = \sqrt{\frac{\lambda_j}{(2\pi)^{d/2}}} \int_{\sum_{i=1}^{d} \lambda_i t_i^2 \leq 1} |t_{j-d}| \exp \left( - \sum_{i=1}^{d} t_i^2 / 2 \right) dx,
\]

\[
\text{Int}_j \geq \frac{\alpha_1^{1/2}}{(2d)^{k/2}} \left( \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} |t_1| e^{-||t||^2/2} dt - \frac{1}{(2\pi)^{d/2}} \int_{||t|| > (d^k/\alpha_2)^{1/2}} |t_1| e^{-||t||^2/2} dt \right).
\]

Here, \( t = [t_1, t_2, \ldots, t_d] \) and \( ||t|| = (\sum_{i=1}^{d} t_i^2)^{1/2} \). The first integral is just \( \sqrt{2/\pi} \). We now show that the second integral goes to zero with \( d \). Indeed, let \( \nu_d \) be for the Gaussian measure on \( \mathbb{R}^d \) with zero mean and the identity covariance operator, and let \( \alpha = (d^k/\alpha_2)^{1/2} \). Then the second integral is \( \int_{\mathbb{R}^d \setminus B_\alpha} |t_1| \nu_d(dt) \), where \( B_\alpha \) denotes the ball of radius \( \alpha \), and is not greater than

\[
\left( \int_{\mathbb{R}^d} t_1^2 \nu_d(dt) \right)^{1/2} (1 - \nu_d(B_\alpha))^{1/2}.
\]

The integral with the integrand \( t_1^2 \) is just one, and using Lemma 2.9.2 from [22] p. 469 we conclude that

\[
1 - \nu_d(B_\alpha) \leq 5 \exp \left( -\alpha^2 / (2d) \right).
\]

Since \( \alpha^2 / (2d) = d^{k-1} \alpha_2 / 2 \) and \( k > 1 \) then this ratio goes to infinity, and \( 1 - \nu_d(B_d) \) goes to zero. This means that \( \text{Int} \) is at least of order \( d^{-k/2} \), and \( I(f) \) is at least of order \( d^{-(k-1)/2} \). Hence to guarantee that \( \hat{I}(f) = I(f) - I(f_d) \leq \xi / 2 \) we must take \( d \) of order \( \varepsilon^{-2/(k-1)} \) which completes the proof for the case \( r = 1 \).

Assume now that \( r \geq 2 \). We first establish an upper bound on \( d(\varepsilon, F_r) \). For \( x = \sum_{j=1}^{\infty} t_j \eta_j \in H \), define \( t = [t_1, t_2, \ldots] \in \mathbb{R}^\infty \) and \( t^d = [t_1, t_2, \ldots, t_d] \). Then we can identify \( f(t) \) with \( f(\text{Im}^{-1} x) \) and \( f(t^d) \) with \( f_d(t) \). By Taylor’s theorem we have

\[
f(t) = f(t^d) + f'(t^d)(t-t^d) + \int_0^1 \left( f'(t^d + u(t-t^d)) - f'(t^d) \right) (t-t^d) du.
\]
Note that \( t - t^d = [0, \ldots, 0, t_{d+1}, t_{d+2}, \ldots] \) and since \( f'(t^d) \) is a linear form we have

\[
f'(t^d)(t - t^d) = \sum_{j=1}^{\infty} a_j t_j,
\]

where \( a_j = a_j(t_1, t_2, \ldots, t_d) \). The mean element of \( \nu \) is zero, which implies that \( I(f'(t^d)(t - t^d)) = 0 \). Hence

\[
I(f) - I(f_d) = I \left( \int_0^1 \left( f'(t^d + u(t - t^d)) - f'(t^d) \right) (t - t^d) \, du \right).
\]

For \( r \geq 2 \), \( f' \) satisfies the Lipschitz condition and we get

\[
|I(f) - I_d(f)| \leq K_2 I \left( \|t - t^d\|^2 \int_0^1 u \, du \right) \\
\leq \frac{K_2}{2} I \left( \sum_{j=d+1}^{\infty} \langle x, \eta_j \rangle_H^2 \right) = \frac{K_2}{2} \sum_{j=d+1}^{\infty} \lambda_j.
\]

For \( \lambda_j = \Theta(j^{-k}) \) we obtain

\[
|I(f) - I_d(f)| = O \left( d^{-(k-1)} \right)
\]

and for \( d = O(\varepsilon^{-1/(k-1)}) \) we guarantee that \( |I(f) - I(f_d)| \leq \frac{\varepsilon}{2} \) for all \( f \in F_r \).

For \( \lambda_j = a_j^{-k} \), we have

\[
\sum_{j=d+1}^{\infty} \lambda_j \leq a \int_d^{\infty} u^{-k} \, du = a \frac{1}{2(k-1)} \frac{1}{d^{k-1}}.
\]

In this case it is enough to take

\[
d = \left\lceil \left( \frac{aK_2}{k-1} \right)^{1/(k-1)} \left( \frac{1}{\varepsilon} \right)^{1/(k-1)} \right\rceil.
\]

For the Wiener measure,

\[
\sum_{j=d+1}^{\infty} \lambda_j \leq \frac{1}{\pi^2} \int_d^{\infty} (u - 1/2)^{-2} \, du = \frac{1}{\pi^2(d - 1/2)},
\]

and

\[
d = \left\lceil \frac{K_2}{\pi^2 \varepsilon} + \frac{1}{2} \right\rceil.
\]

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This establishes upper bounds on $d(\varepsilon, F_r)$.

To get a lower bound, consider the function $g(x) = c_r x^2/(1 + x^2) = c_r (1 - 1/(1 + x^2))$ for $x \in \mathbb{R}$, where $c_r$ is a positive number chosen such that $\max_{0 \leq i \leq r-1} \sup_{x \in \mathbb{R}} |g^{(i)}(x)|/K_i \leq 1$, and such that $g^{(r-1)}$ satisfies the Lipschitz condition with the constant $K_r$. It is easy to see that such a positive number $c_r$ exists. Indeed, the $j$th derivatives of $1/(1 + x^2)$ can be written as the ratio of two polynomials $p_j(x)/(1 + x^2)^{j+1}$ with the degree of $p_j$ being at most $j$, and therefore all derivatives go to zero as $|x|$ goes to infinity.

As for the case $r = 1$, we take $x_d = \sum_{j=d+1}^{2d} \langle x, \eta_j \rangle_{H^j}$, and $f(\text{Im}^{-1} x) = g(\|x_d\|)$. Then $f \in F_r, f_d = 0$ and $I(f) - I(f_d) = I(f)$. Similarly as for $r = 1$ we have

$$I(f) \geq \frac{c_r \lambda_2 d}{2} \int_{\|t\| \leq \alpha} \|t\|^2 \nu_d(dt),$$

where $\alpha = (d^k/\alpha_2)^{1/2}$. We now show that the last integral tends to $d$. Indeed, it can be written as

$$\int_{\mathbb{R}^d} \|t\|^2 \nu_d(dt) - \int_{\|t\| > \alpha} \|t\|^2 \nu_d(dt).$$

The first integral is obviously $d$, and we show that the integral over the outside of the ball tends to zero. For large $d$, the norm of $t$ is also large, and we can estimate $\|t\|^2 \leq \exp(c_d \|t\|^2/2)$ for $c_d = 2\alpha_2 \ln(d^k/\alpha_2)/d^k$. Then

$$\int_{\|t\| > \alpha} \|t\|^2 \nu_d(dt) \leq (1 - c_d)^{d/2} \int_{\|t\| > \alpha} \nu_{d,c}(dt),$$

where $\nu_{d,c}$ is a Gaussian measure on $\mathbb{R}^d$ with mean zero and covariance operator $(1 - c_d)^{-1}I$. Again using Lemma 2.9.2 from [22] we obtain

$$\int_{\|t\| > \alpha} \|t\|^2 \nu_d(dt) \leq 5(1 - c_d)^{d/2} \exp\left(-\alpha^2(1 - c_d)/d\right).$$

Since $k > 1$, the quantity $(1 - c_d)^d$ tends to 1, and since $\alpha^2/d = \Theta(d^{k-1})$ tends to infinity, the integral goes to zero as claimed.

Hence, $I(f)$ is at least of order $d^{-(k-1)}$ and $d$ must be at least of order $\varepsilon^{-1/(k-1)}$ to guarantee $I(f) \leq \frac{\varepsilon}{2}$. This completes the proof for $r \geq 2$.

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