Eigenvector Approximation Leading to Exponential Speedup of Quantum Eigenvalue Calculation

Peter Jaksch* and Anargyros Papageorgiou†

Department of Computer Science, Columbia University, New York, New York 10027-6902, USA

(Received 26 March 2003; published 19 December 2003)

We present an efficient method for preparing the initial state required by the eigenvalue approximation quantum algorithm of Abrams and Lloyd. Our method can be applied when solving continuous Hermitian eigenproblems, e.g., the Schrödinger equation, on a discrete grid. We start with a classically obtained eigenvector for a problem discretized on a coarse grid, and we efficiently construct, quantum mechanically, an approximation of the same eigenvector on a fine grid. We use this approximation as the initial state for the eigenvalue estimation algorithm, and show the relationship between its success probability and the size of the coarse grid.

DOI: 10.1103/PhysRevLett.91.257902 PACS numbers: 03.67.Lx, 02.60.–x

Intuitively, quantum mechanical problems offer great potential for quantum computers to achieve large speedups over classical machines. An important problem of this kind is the approximation of an eigenvalue of a quantum mechanical evolution operator. In a recent paper [1], Abrams and Lloyd present a quantum algorithm for doing this. Their algorithm is exponentially faster than the best classical algorithm, but requires a good approximation of an eigenvector as input. In this Letter, we show how to obtain an approximation efficiently which is guaranteed to be good.

The key component of the algorithm in [1] is quantum phase estimation, which is a method for approximating an eigenvalue of a unitary matrix [2]. We give a brief outline of this algorithm below.

Let Q denote a $2^m \times 2^m$ unitary matrix. We want to approximate a specific eigenvalue of Q. Phase estimation does this using the corresponding eigenvector as input. The algorithm in [1] deals with the case when this eigenvector is not known exactly. In particular, consider a quantum computer consisting of three registers with a total of $b + m + w$ qubits. The first b qubits are all initially in the state $|0\rangle$. The second register with m qubits is initialized to some state $|\psi\rangle$, which must approximate the eigenvector in question sufficiently well, as we will see. The last w qubits are work qubits for temporary storage.

Since Q is unitary and therefore normal, the state $|\psi\rangle$ can be expanded with respect to eigenvectors of Q. Omitting the work qubits, the initial state of the algorithm is

$$|0\rangle|\psi\rangle = |0\rangle\sum_u d_u|u\rangle, \tag{1}$$

where $|u\rangle$ are the eigenvectors of Q. Placing the first register in an equal superposition, using b Hadamard gates, transforms this state into

$$\frac{1}{\sqrt{2^b}}\sum_{j=0}^{2^b-1}|j\rangle\sum_u d_u|u\rangle. \tag{2}$$

Next, powers of Q are applied to create the state

$$\frac{1}{\sqrt{2^b}}\sum_{j=0}^{2^b-1}|j\rangle Q^j\sum_u d_u|u\rangle. \tag{3}$$

Since Q is unitary, its eigenvalues can be written as $e^{2\pi i\varphi_u}$, where $\varphi_u \in R$. We can assume that $\varphi_u \in [0, 1)$ and consider the approximation of one of these phases instead of the approximation of one of the eigenvalues. Equation (3) is equal to

$$\frac{1}{\sqrt{2^b}}\sum_u\sum_{j=0}^{2^b-1} d_u e^{2\pi i j\varphi_u}|j\rangle|u\rangle. \tag{4}$$

It is easily seen that the inverse Fourier transform performed on the first register creates the state

$$\sum_u d_u\left(\sum_{j=0}^{2^b-1} g(\varphi_u, j)|j\rangle\right)|u\rangle, \tag{5}$$

where

$$g(\varphi_u, j) = \begin{cases} \frac{\sin[\pi(2^b\varphi_u - j)]e^{\pi i(\varphi_u - j2^{-b})(2^b-1)}}{2^b\sin[\pi(\varphi_u - j2^{-b})]}, & 2^b\varphi_u \neq j \\ 1, & 2^b\varphi_u = j. \end{cases} \tag{6}$$

A measurement of the first register produces outcome j with probability

$$p_j = \sum_u |d_u|^2|g(\varphi_u, j)|^2, \tag{7}$$

and the second register will collapse to the state

$$\sum_u \frac{d_u g(\varphi_u, j)}{\sqrt{p_j}}|u\rangle. \tag{8}$$

We remark that, for the special case when the eigenvalues φ_u can be represented exactly with b bits (i.e., $2^b\varphi_u$ is an integer), Eq. (5) simplifies to

$$\sum_u d_u |\varphi_u\rangle |u\rangle. \quad (9)$$

Thus, when the eigenvalues are of this form, and are distinct, a measurement of the first register will cause the second register to collapse exactly onto the corresponding eigenvector.

Recall that we are interested in approximating the phase that corresponds to an eigenvector $|u'\rangle$, that the state $|\psi\rangle$ is an approximation of this eigenvector, and that the eigenvalue is of the form $e^{2\pi i \varphi_{u'}}$. For instance, one is often interested in the eigenvalue corresponding to the ground state. We define $\Delta(\varphi_0, \varphi_1) = \min_{x \in Z}\{|x + \varphi_1 - \varphi_0|\}$, $\varphi_0, \varphi_1 \in R$ (i.e., the fractional part of the distance between φ_0 and φ_1). Then a measurement of the first register produces an outcome from the set $\mathcal{G} = \{j : \Delta(j/2^b, \varphi_{u'}) \le k/2^b,\ k > 1\}$ with probability

$$\Pr(\mathcal{G}) = \sum_{j \in \mathcal{G}} \sum_u |d_u g(\varphi_u, j)|^2 \ge \sum_{j \in \mathcal{G}} |d_{u'} g(\varphi_{u'}, j)|^2$$

$$\ge |d_{u'}|^2 - \frac{|d_{u'}|^2}{2(k-1)}, \quad (10)$$

and when $k = 1$ the probability that $\Delta(j/2^b, \varphi_{u'}) \le 2^{-b}$ is bounded from below by $(8/\pi^2)|d_{u'}|^2$, where the proofs of the probability bounds can be found in [2,3]. Observe that $|\psi\rangle$ must be chosen in a way that this probability is greater than $\frac{1}{2}$, which implies that $|d_{u'}|$ has to be sufficiently large. If we want to obtain an approximation of $\varphi_{u'}$ with accuracy 2^{-n} and probability at least $|d_{u'}|^2(1 - \epsilon)$, Eq. (10) shows that this can achieved by choosing the number of qubits b in the first register to be

$$b = n + \left\lceil \log\left(1 + \frac{1}{2\epsilon}\right) \right\rceil. \quad (11)$$

The algorithm in [1] is based on the fact that quantum phase estimation can be used as an efficient subroutine to find eigenvalues. Consider a Hermitian operator H. The operator $G(t) = e^{-iHt}$ is unitary and has the same eigenvectors as H. We assume that G can be implemented efficiently and, therefore, can be used as the unitary operator in the phase estimation algorithm. For example, when H is local, i.e., it can be written in the form $\sum H_j$, where each H_j acts only on a small number of qubits, then G can be implemented efficiently as shown in [4] (for more details, see [1] and the references therein). However, locality is not a necessary condition for efficient implementation. Indeed, Zalka [5] shows that G can be efficiently implemented for a many-particle quantum mechanical system with a nonlocal H. Nielsen and Chuang [2], on page 210, also state that it is possible to implement G for a wide class of nonlocal Hamiltonians, and give an example of one such Hamiltonian.

The Hermitian eigenproblem described above is solved on a discrete grid. We are interested in the case when the grid is extremely fine. Clearly, a fine grid requires a large vector for the representation of the initial state of the algorithm. In general, it may not be possible to efficiently prepare an arbitrary quantum state in a space with a large number of qubits. However, in our case we will show a method for the efficient preparation of an initial state.

Suppose we have an eigenvector for a coarse grid discretization of the problem. We can assume that we obtained it classically because the size of the problem is small. Using this eigenvector, we efficiently construct an approximation to the corresponding eigenvector for a fine grid discretization of the problem. We use this approximation as the initial state of the eigenvalue approximation algorithm. We describe our method for a one-dimensional continuous problem on the interval $[0, 1]$.

Let H be a positive Hermitian operator, defined on a Hilbert space of smooth functions on $[0, 1]$. Let $v_k(\cdot)$, $k = 1, 2, \ldots$ denote the eigenfunctions of H, ordered according to the magnitude of the corresponding eigenvalues; without loss of generality, we assume that

$$\int_0^1 |v_k(x)|^2 \, dx = 1. \quad (12)$$

Suppose that H_N is a discretization of H with grid size $h_N = 1/(1 + N)$. Let $|U_k^{(N)}\rangle$, $k = 0, 1, \ldots, N - 1$ denote the normalized eigenvectors of H_N, ordered according to the magnitude of the corresponding eigenvalues. The expansion of the kth eigenvector in the computational basis can be written as

$$|U_k^{(N)}\rangle = \sum_{j=0}^{N-1} u_{k,j}^{(N)} |j\rangle. \quad (13)$$

Let $|V_k^{(N)}\rangle = \sum_{j=0}^{N-1} v_k[(j + 1)h_N]|j\rangle$ be the sampled version of $v_k(\cdot)$ at the discretization points. Consider problems such that the eigenvector of interest satisfies $\|v_k'\|_\infty = \sup_{0 \le x \le 1} |v_k'(x)| = O(1)$ and

$$\left\| |U_k^{(N)}\rangle - \frac{|V_k^{(N)}\rangle}{|V_k^{(N)}\rangle} \right\| = O(h_N^q), \quad (14)$$

where $q > 0$ is the order of convergence and $\||X\rangle\|^2 = \sum_{j=0}^{N-1} |x_j|^2$, for $|X\rangle = \sum_{j=0}^{j=N-1} x_j |j\rangle$. For example, these conditions are satisfied when we are dealing with second order elliptic operators; see [6] for the solution of eigenvalue problems.

Now, assume that the eigenvector $|U_k^{(N_0)}\rangle$ of H_{N_0} has been obtained classically [7]. This vector is placed in a $\log N_0$ qubit register. For $N = 2^s N_0$, we construct an approximation $|\tilde{U}_k^{(N)}\rangle$ of $|U_k^{(N)}\rangle$ by appending s qubits, in the state $|0\rangle$, to $|U_k^{(N_0)}\rangle$, and then performing a Hadamard transformation on each one of these s qubits; i.e.,

$$|\tilde{U}_k^{(N)}\rangle = |U_k^{(N_0)}\rangle \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}} \right)^{\otimes s} = \frac{1}{\sqrt{2^s}} \sum_{j=0}^{N-1} u_{k,f(j)}^{(N_0)} |j\rangle, \quad (15)$$

where $f(j) = \lfloor j/2^s \rfloor$. The effect of f is to replicate the

coordinates of $|U_k^{(N_0)}\rangle$ 2^s times. We use $|\tilde{U}_k^{(N)}\rangle$ as input to the eigenvalue and eigenvector approximation algorithm. When the result of the algorithm is measured, $|\tilde{U}_k^{(N)}\rangle$ will collapse onto a superposition of eigenvectors according to Eq. (8). We show that the magnitude of the coefficient of $|U_k^{(N)}\rangle$ in this superposition can be made arbitrarily close to 1 by appropriately choosing N_0.

Consider two different expansions of $|\tilde{U}_k^{(N)}\rangle$:

$$|\tilde{U}_k^{(N)}\rangle = \sum_{j=0}^{N-1} \tilde{u}_{k,j}^{(N)} |j\rangle, \tag{16}$$

$$|\tilde{U}_k^{(N)}\rangle = \sum_{l=0}^{N-1} d_{k,l}^{(N)} |U_l^{(N)}\rangle. \tag{17}$$

The first expansion is in the computational basis and the second is with respect to the eigenvectors of H_N. We call $|d_{k,k}^{(N)}|^2$ the probability of success. Equation (17) can be rewritten as

$$|\tilde{U}_k^{(N)}\rangle - |U_k^{(N)}\rangle = (d_{k,k}^{(N)} - 1)|U_k^{(N)}\rangle + \sum_{l\neq k} d_{k,l}^{(N)} |U_l^{(N)}\rangle. \tag{18}$$

Taking norms on both sides and using (13) and (16) gives the inequality

$$\begin{aligned} \| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \|^2 &= \sum_{j=0}^{N-1} |u_{k,j}^{(N)} - \tilde{u}_{k,j}^{(N)}|^2 \\ &= |d_{k,k}^{(N)} - 1|^2 + \sum_{l\neq k} |d_{k,l}^{(N)}|^2 \geq \sum_{l\neq k} |d_{k,l}^{(N)}|^2 \\ &= 1 - |d_{k,k}^{(N)}|^2. \end{aligned} \tag{19}$$

We will now bound (19) from above, and thus the probability of failure. The definition of $|\tilde{U}_k^{(N)}\rangle$ implies

$$\| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \|^2 = \sum_{j=0}^{N-1} \left| \frac{v_k[(j+1)h_N]}{\| |V_k^{(N)}\rangle \|} - \frac{v_k\{[f(j)+1]h_{N_0}\}}{\sqrt{2^s}\| |V_k^{(N_0)}\rangle \|} + \Delta_{k,j}^{(N)} - \frac{\Delta_{k,f(j)}^{(N_0)}}{\sqrt{2^s}} \right|^2, \tag{20}$$

where $\sum_{j=0}^{N-1} |\Delta_{k,j}^{(N)}|^2 = O(h_N^{2q})$ and $\sum_{j=0}^{N-1} |\Delta_{k,f(j)}^{(N_0)}|^2 = 2^s O(h_{N_0}^{2q})$ by (14). Applying the triangle inequality, we get

$$\| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \| \leq \left(\sum_{j=0}^{N-1} \left| \frac{v_k[(j+1)h_N]}{\| |V_k^{(N)}\rangle \|} - \frac{v_k\{[f(j)+1]h_{N_0}\}}{\sqrt{2^s}\| |V_k^{(N_0)}\rangle \|} \right|^2 \right)^{1/2} + O(h_{N_0}^q). \tag{21}$$

The definition of $|V_k^{(N)}\rangle$ and the fact that $\|v_k'\|_\infty = O(1)$ imply that $\| |V_k^{(N)}\rangle \| = \sqrt{N}[1 + O(h_N)]$. Hence, the sum above is equal to

$$\begin{aligned} \frac{1}{N} \sum_{j=0}^{N-1} |v_k[(j+1)h_N][1 + O(h_N)] \\ - v_k\{[f(j)+1]h_{N_0}\}[1 + O(h_{N_0})]|^2. \end{aligned} \tag{22}$$

Since $v_k(\cdot)$ is continuous with a bounded first derivative, we have that

$$v_k(x_{2,j}) = v_k(x_{1,j}) + O(|x_{2,j} - x_{1,j}|), \tag{23}$$

where $x_{1,j} = (j+1)h_N$ and $x_{2,j} = [f(j)+1]h_{N_0}$, $j = 0, \ldots, N-1$. Clearly $|x_{2,j} - x_{1,j}| = O(h_{N_0})$. Using (22), (23), and the triangle inequality, we obtain from (21) that

$$\begin{aligned} \| |U_k^{(N)}\rangle - |\tilde{U}_k^{(N)}\rangle \| &\leq O(h_{N_0}) \frac{\| |V_k^{(N)}\rangle \|}{\sqrt{N}} + O(h_{N_0}) + O(h_{N_0}^q) \\ &= O(h_{N_0}^{\min\{1,q\}}). \end{aligned} \tag{24}$$

Hence, the probability of failure is bounded from above by $O(N_0^{-\min\{2,2q\}})$. It depends only on the order of convergence to the continuous problem and the number of points in the classically solved small problem. We can select an N_0 such that the probability of failure is less than $1/2$, no matter how much larger N is. By choosing a large N, we can make the discretization error arbitrarily small. Equation (24) implies that the probability of obtaining the eigenvalue $e^{2\pi i \varphi_k}$ with accuracy 2^{-b} is at least $(8/\pi^2)[1 - O(N_0^{-\min\{2,2q\}})]$.

We remark that any classical numerical algorithm that computes an eigenvalue, satisfying a specific (nontrivial) property, of a $N \times N$ unitary matrix takes time $\Omega(N)$. For example, one may want to find the eigenvalue that corresponds to the ground state. This is true even if a matrix is sparse and regardless of whether the algorithm is deterministic or randomized. It is merely a consequence of the fact that the algorithm needs to consider all the (nonzero) elements of the matrix, and there are at least $\Omega(N)$ of them. Alternatively, in the restricted case when the matrix is diagonal, finding one of its elements is a problem at least as hard as searching an unordered list. The lower bound for searching yields the lower bound in our case.

In conclusion, our method provides a highly efficient preparation of initial states for eigenvalue approximation, requiring only a small number of Hadamard gates. Thus, the algorithm of Abrams and Lloyd, using our initial state, computes the eigenvalue exponentially faster than any classical algorithm. The method can be generalized to higher dimensional continuous problems. This will be the subject of a future paper.

This research was supported in part by U.S. Air Force, Air Force Material Command, Air Force Research Laboratory/IFKF, under Contract No. F30602-01-0523. P. J. also acknowledges support from the foundation Blanceflor Boncompagni-Ludovisi, née Bildt. We are grateful to Joseph Traub and Arthur Werschulz for helpful discussions and valuable comments.

*Electronic address: petja@cs.columbia.edu
†Electronic address: ap@cs.columbia.edu

[1] D. S. Abrams and S. Lloyd, Phys. Rev. Lett. **83**, 5162 (1999).
[2] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
[3] G. Brassard, P. Hoyer, M. Mosca, and A. Tapp, *Quantum Amplitude Amplification and Estimation*, in Contemporary Mathematics Vol. 305 (American Mathematical Society, Providence, 2002), pp. 53–74, available at Los Alamos eprint archive as http://arXiv.org/abs//quant-ph/0005055.
[4] S. Lloyd, Science **273**, 1073 (1996).
[5] C. Zalka, in Proc. R. Soc. London A **454**, 313 (1998).
[6] I. Babuska and J. Osborn, in *Handbook of Numerical Analysis*, edited by P. G. Ciarlet and J. L. Lions (North-Holland, Amsterdam, 1991), Vol. II, pp. 641–787.
[7] In fact, we can weaken this condition by considering the numerical error in solving the coarsely discretized problem. It suffices to assume that we have an approximation $|\hat{U}_k^{(N_0)}\rangle$ of the eigenvector $|U_k^{(N_0)}\rangle$ such that $\||\hat{U}_k^{(N_0)}\rangle - |U_k^{(N_0)}\rangle\| = O(h_{N_0}^q)$.