International Journal of Quantum Information
Vol. 14, No. 1 (2016) 1650005 (14 pages)

DOI: 10.1142/S0219749916500052

Quantum eigenvalue estimation for irreducible non-negative matrices

Anmer Daskin

Department of Computer Engineering
Istanbul Medeniyet University
Uskudar, Istanbul, Turkey
anmerdaskin@yahoo.com

Received 20 November 2015
Revised 29 February 2016
Accepted 2 March 2016
Published 27 April 2016

Quantum phase estimation algorithm (PEA) has been successfully adapted as a sub frame of many other algorithms applied to a wide variety of applications in different fields. However, the requirement of a good approximate eigenvector given as an input to the algorithm hinders the application of the algorithm to the problems where we do not have any prior knowledge about the eigenvector. In this paper, we show that the principal eigenvalue of an irreducible non-negative operator can be determined by using an equal superposition initial state in the PEA. This removes the necessity of the existence of an initial good approximate eigenvector. Moreover, we show that the success probability of the algorithm is related to the closeness of the operator to a stochastic matrix. Therefore, we draw an estimate for the success probability by using the variance of the column sums of the operator. This provides *a priori* information which can be used to know the success probability of the algorithm beforehand for the non-negative matrices and apply the algorithm only in cases when the estimated probability is reasonably high. Finally, we discuss the possible applications and show the results for random symmetric matrices and 3-local Hamiltonians with non-negative off-diagonal elements.

Keywords: Quantum phase estimation; non-negative matrices; eigenvalue estimation.

1. Introduction

In the recent decades, quantum algorithms are shown to be more efficient for some problems than their classical counterparts.[1,2] The quantum phase estimation[3–6] is a leading illustration of such algorithms. In the simulation of quantum systems, the algorithm is used to estimate the eigenenergy corresponding to a given approximate eigenvector of a quantum Hamiltonian operator (e.g. Refs. 7–16). Furthermore, it has been adapted as a sub frame of algorithms applied to a wide variety of applications in different fields (see the review article Ref. 17 and the references therein). It is known

that the initial approximation to the eigenvector associated with the desired eigenvalue plays important role in the success of the algorithm: the phase estimation algorithm (PEA) mainly uses two quantum registers for the eigenvalue and the eigenvector. In the initial step, while the first register, $|reg1\rangle$, is set to zero state, the second register, $|reg_2\rangle$, holds an approximate eigenvector associated to the desired eigenvalue. The initial state of $|reg_2\rangle$ affects the success probability of finding the desired eigenvalue in the first register. Therefore, despite the ubiquitous use of the algorithm, it may fail in the cases where the initial approximation to the eigenvector is not good enough. This hinders the application of the algorithm when there is not enough prior knowledge to procure a good approximation to the eigenvector. Assuming there is no known approximate eigenvector, in this article, we investigate the applications of the algorithm to irreducible non-negative matrices.

A symmetric matrix is called non-negative if all of its elements are greater than or equal to zero. It is irreducible if the corresponding graph is strongly connected or if it is not reducible to a block-diagonal form by any column–row permutation. Due to Perron–Frobenius theorem,[18] an irreducible non-negative matrix have a positive eigenvector (all elements are positive) with an associated positive principal eigenvalue whose magnitude is greater than the rest of the eigenvalues. These matrices have been studied extensively.[19,20] In addition, the distribution and the sum of the coefficients of their principal eigenvectors have been shown to be related to the matrix elements[21] and the number of walks in molecular graphs,[22] respectively.

We show that for irreducible non-negative matrices, one can obtain the principal eigenvalue by using an equal superposition input state in PEA i.e. instead of an approximate eigenvector, initial value of $|reg_2\rangle$ is set to the zero state, $|\mathbf{0}\rangle$, and then put into the equal superposition state by applying Hadamard gates. In the end, these initial settings generate a superposition of the eigenvalues with the probabilities determined by the normalized sums of the coefficients of the eigenvectors. Because all of the eigenvectors, but the principal one, include positive–negative elements, we find that the probability to see the principal eigenvalue is much greater than the others in most of the random cases. Also, in some cases, we show that the success probability can be further increased by applying the following measurement scheme:

- Hadamard gates are applied to the second register in the output. (or the second register can be measured in the Hadamard basis.)
- Then, the first register is measured when the second register is found in the state $|\mathbf{0}\rangle$.

Moreover, we present an attempt to estimate the success probability of the algorithm for an irreducible non-negative matrix by using its closeness to a stochastic matrix: since the eigenvector-coefficients of a stochastic matrix sum to zero for all but the principal eigenvector, one can generate the principal eigenvalue of the matrix in PEA with probability one.[23] Any given symmetric irreducible

non-negative matrix can be converted into a stochastic matrix by a diagonal scaling matrix. This diagonal matrix together with the matrix norm is used to derive a formula to predict the success probability of the algorithm. We finally compare the estimated success probabilities with the computed ones for random symmetric matrices and 3-local Hamiltonians of different dimensions with non-negative off-diagonal elements.

In the following sections, after PEA is given in detailed steps, the estimation of the success probability is discussed. In the final sections, the possible applications and numerical results are presented.

2. Quantum Phase Estimation Algorithm

PEA in general sense finds the value of the phase, ϕ_j, for a given approximate eigenvector $|\mu_j\rangle$ in the eigenvalue equation $U|\mu_j\rangle = e^{i\phi_j}|\mu_j\rangle$. As noted in the previous section, the algorithm uses two quantum registers: viz. $|reg_1\rangle$ initially set to zero state and $|reg_2\rangle$ holding an approximate eigenstate of a unitary matrix U. The first operation in the algorithm, the quantum Fourier transform (QFT), puts $|reg_1\rangle$ into the equal superposition state. In this setting, a sequence of operators, $U^{2^{j-1}}$s, controlled by the jth qubit of $|reg_1\rangle$ are applied to $|reg_2\rangle$. Here, $j = 1 \ldots m$ and m is the number of qubits in $|reg_1\rangle$ and so determines the precision of the output.These sequential operations generate the QFT of the phase on $|reg1\rangle$. Therefore, the application of the inverse QFT† turns the value of $|reg1\rangle$ into the binary value of the phase. Consequently, one measures $|reg_1\rangle$ to obtain the phase. Here, if the unitary operator U is the time evolution operator of a quantum Hamiltonian $\mathcal{H}$, i.e. $U = e^{i\mathcal{H}}$; then one also obtains the eigenenergy of that Hamiltonian.

For a symmetric irreducible non-negative matrix $\mathcal{H}$ of order $N = 2^n$ with ordered eigenvalues as $\phi_1 \geq \cdots \geq \phi_N$ and associated eigenvectors $|\mu_1\rangle \ldots |\mu_N\rangle$, it is known that $|\mu_1\rangle$ is the only eigenvector with all positive coefficients. Assume unitary operator $U = e^{i\mathcal{H}}$ and its powers $U^{2^{j-1}}$ with $j = 1 \ldots m$ are readily available for PEA. To estimate the value of ϕ_1 on the first register, in our setting, we simply modify the conventional phase estimation algorithm in the following way:

- Instead of an approximate eigenvector, initial value of $|reg_2\rangle$ is set to $|\mathbf{0}\rangle$ and then put into equal superposition state by applying Hadamard gates.
- (**optional**) In the output, we change the basis of the second register by applying the Hadamard gates. Then, if the measurement of the second register is equal to $|\mathbf{0}\rangle$ state, then the principal eigenvalue is estimated on the first register. This modification increases the success probability of the algorithm further when the probability of measuring the principal eigenvalue is higher than the other eigenvalues.

In the following subsection, the phase estimation shall be described in steps to explicitly show the impacts of the above modifications on the algorithm. These steps are also depicted in Fig. 1.

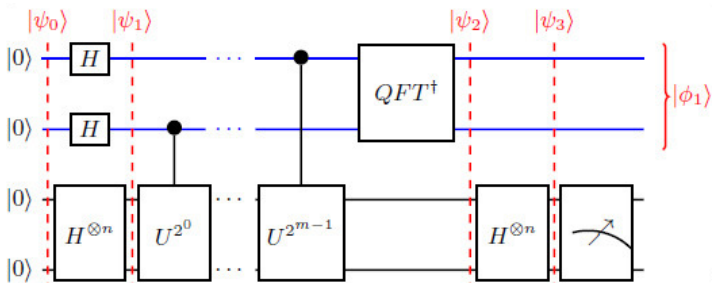


Fig. 1. Circuit design for the modified phase estimation algorithm. In the end, note that the application of the Hadamard gates to the second register and the measurement on this register are optional.

2.1. *Steps of the algorithm*

Here, the algorithm is described in details by showing how the quantum state changes in each step:

- The system is prepared in a way so that it includes two registers: viz. $|reg_1\rangle$ and $|reg_2\rangle$ with m and n number of qubits, respectively.
- Both registers are initialized into zero state: $|\psi_0\rangle = |reg_1\rangle|reg_2\rangle = |\mathbf{0}\rangle|\mathbf{0}\rangle$.
- Then, the Hadamard operators are applied to both registers:

$$|\psi_1\rangle = (H^{\otimes m} \otimes H^{\otimes n})|\mathbf{0}\rangle|\mathbf{0}\rangle = \frac{1}{\sqrt{2^{n+m}}} \sum_{x=0}^{2^{m+n}-1} |\mathbf{x}\rangle, \tag{1}$$

  where $|\mathbf{x}\rangle$ is the xth vector in the standard basis.
- As in the customary phase estimation algorithm; the unitary evolution operators $U^{2^{j-1}}$ controlled by the jth qubit of $|reg_1\rangle$ are applied to $|reg_2\rangle$. And finally the inverse of the QFT† is applied to $|reg1\rangle$.

  At this point of the algorithm, we have a quantum state in which $|reg_1\rangle$ and $|reg_2\rangle$ hold the superposition of the eigenvalues and the associated eigenvectors, respectively:

$$|\psi_2\rangle = \sum_{j=1}^{N} \alpha_j |\phi_j\rangle|\mu_j\rangle. \tag{2}$$

  Here, the amplitude α_j is related to the angle (overlap) between the equal superposition state, $1/\sqrt{N}\sum_{x=0}^{N-1}|\mathbf{x}\rangle$, and the eigenvector $|\mu_j\rangle$. Therefore, α_j describes the normalized sum of the coefficients of $|\mu_j\rangle$:

$$\alpha_j = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \mu_{ji}. \tag{3}$$

If we rewrite $|reg_2\rangle$ in the Hadamard basis, we obtain the following:

$$|\psi_2\rangle = \sum_{j=1}^{N} \beta_{1j}|\phi_j\rangle|+\cdots+\rangle + \cdots + \sum_{j=1}^{N} \beta_{Nj}|\phi_j\rangle|-\cdots-\rangle, \tag{4}$$

where $|\pm\rangle = 1/\sqrt{(}2)(|0\rangle \pm |1\rangle)$ and β_{ij}s are new coefficients. Now, since there is only one eigenvector with all positive real elements, i.e. $|\mu_1\rangle$, in the Hadamard basis, we can expect this positive eigenvector to be the closest state to $|+\cdots+\rangle$.

- To revert the above state back to the standard basis, the Hadamard operator $H^{\otimes n}$ is again applied to $|reg_2\rangle$:

$$\begin{aligned} |\psi_3\rangle &= (I \otimes H^{\otimes n})|\psi_2\rangle \\ &= \sum_{j=1}^{N} \beta_{1j}|\phi_j\rangle|0\cdots0\rangle + \cdots + \sum_{j=1}^{N} \beta_{Nj}|\phi_j\rangle|1\ldots1\rangle, \end{aligned} \tag{5}$$

- $|reg_2\rangle$ is measured in the standard basis. As a result, for $|reg_2\rangle = |0\ldots00\rangle$, the system collapses to the state where the phase associated with the positive eigenvector is expected to be highly dominant in the first register.
- In the final step, the first register is measured to obtain the phase ϕ_1 and get the eigenvalue of $\mathcal{H}$.

2.2. *The success probability*

It is easy to see that the success probability of the algorithm without the optional Hadamard gates on $|reg_2\rangle$ in the output is determined from the normalized sum of the coefficients of the eigenvectors given in Eq. (3). Therefore, the success probability for the dominant eigenvalue is α_1^2 which is the normalized sum of the coefficients of $|\mu_1\rangle$ (note that since the coefficients of $|\mu_1\rangle$ are positive, $\alpha_1^2 = |\alpha_1|^2$).

With the Hadamard gates in the output, we first find the probability to measure $|reg_2\rangle$ in $|\mathbf{0}\rangle$ state and then find the probability to see the dominant eigenvalue in $|reg_1\rangle$ knowing $|reg_2\rangle = |\mathbf{0}\rangle$: from Eq. (5), we can observe that the probability to see $|\mathbf{0}\rangle$ on $|reg_2\rangle$ is $|\sum_{j=1}^{N} \beta_{1j}|^2$. Therefore, the conditional probability, the probability to measure $|\phi_1\rangle$ on $|reg_1\rangle$ when $|reg_2\rangle$ is $|\mathbf{0}\rangle$, is described by $|\beta_{11}|^2$.

Since we use the equal superposition state as an input, the sum of the components of an eigenvector has determined the probability to get the corresponding eigenvalue on $|reg_1\rangle$, which is found in Eq. (2). If we measure $|reg_2\rangle$ in Eq. (2) in the Hadamard basis, the probability to see $|reg_2\rangle = |+\cdots+\rangle$ is again determined by the sum of the components of the eigenvectors since $|+\cdots+\rangle = 1/\sqrt{N}\sum_{x=1}^{N}|\mathbf{x}\rangle$. For instance, the probability to see $|\phi_j\rangle$ on $|reg_1\rangle$ and $|+\cdots+\rangle$ on $|reg_2\rangle$ becomes $|\alpha_j|^4$. Therefore, without including the first register, the total probability to see $|+\cdots+\rangle$ on $|reg_2\rangle$ is

$$P_{reg_2} = \sum_{j=1}^{N} |\alpha_j|^4 \geq \frac{1}{N}. \tag{6}$$

This is also equal to $\sum_{j=1}^{N} \beta_{1j}$, i.e. the probability of measuring $|reg_2\rangle$ in $|0 \dots 0\rangle$ state at the end. P_{reg_2} takes the smallest value only when all $|\alpha_j|$s are equal to $1/\sqrt{N}$.

As a result, when $|reg_2\rangle = |0 \cdots 0\rangle$, the probability to see $|\phi_1\rangle$ on $\rangle reg_1\langle$ is:

$$P_{reg_1} = |\beta_{11}|^2 = \frac{\alpha_1^4}{P_{reg_2}}. \tag{7}$$

2.2.1. *Estimation of the success probability*

Although we have drawn the equalities for probabilities, without knowing the eigenvectors, it is not possible to compute exact $|\alpha_j|$s and so P_{reg_1} and P_{reg_2}. Therefore, we shall try to estimate them: since α_1 is the normalized sum of the vector elements, it is easy to see that $\alpha_1 \geq 1/\sqrt{N}$, where the equality occurs only when the magnitude of the eigenvectors are the columns of the identity matrix. A similar observation is also made in Ref. 23 where the principal eigenvector is found for a given eigenvalue equal to one.

To develop some intuition for the estimation of the probabilities, we will relate the matrix $\mathcal{H}$ to a stochastic matrix. It is known that stochastic matrices have only one eigenvector with coefficients summing to a non-zero value. A matrix can be made stochastic by a column wise scaling $\mathcal{HD}$, where $\mathcal{D}$ is a diagonal matrix whose diagonal elements are the inverses of the sums of the columns of $\mathcal{H}$. The closeness of the matrix $\mathcal{H}$ to $\mathcal{HD}$ may provide a prediction to estimate the success behavior of the PEA with an initial superposition state. The closeness of $\mathcal{H}$ to $\mathcal{HD}$ can be defined by $||\mathcal{H} - \mathcal{HD}||$ where $||\cdot||$ is any matrix norm. This also defines a perturbation error. If we normalize this error term by $||\mathcal{H}||$, we get the relative error:

$$\epsilon_1 = \frac{||\mathcal{H} - \mathcal{HD}||}{||\mathcal{H}||} \leq ||\mathcal{I} - \mathcal{D}||, \tag{8}$$

where $\mathcal{I}$ is an identity matrix. We can also look at the relative error in the inverses:

$$\epsilon_1 = \frac{||\mathcal{H}^{-1} - \mathcal{D}^{-1}\mathcal{H}^{-1}||}{||\mathcal{H}^{-1}||} \leq ||\mathcal{I} - \mathcal{D}^{-1}||. \tag{9}$$

Since the matrix $\mathcal{D}$ also changes the eigenvector elements; when the variance of the diagonal elements of $\mathcal{D}$ is small, we can expect the eigenvectors of $\mathcal{H}$ to exhibit the similar behaviors as of $\mathcal{HD}$ and have one eigenvector whose elements sum to a much greater value than the others. When $\mathcal{H} = \mathcal{HD}$ or $\mathcal{D} = \mathcal{I}$, left and right principal eigenvectors of symmetric $\mathcal{H}$ are the same and have the elements equal to $\frac{1}{\sqrt{N}}$ in the normalized space. Therefore, the variances σ_1 and σ_2 of the diagonal elements of $\mathcal{D}^{-1}$ and $\mathcal{D}$, the column sums of $\mathcal{H}$ and their inverses, can somehow describe how much the elements of the principal eigenvector deviate from $\frac{1}{\sqrt{N}}$ which is also the expectation value for randomly generated normalized uniform N numbers. Using these intuitions, we define the estimate of P_{reg_2} as:

$$\tilde{P}_{reg_2} = \frac{\Lambda_1 + \Lambda_2}{2} \tag{10}$$

with

$$\Lambda_1 = \frac{\frac{1}{N} - \sigma_1}{\frac{1}{N} + \sigma_1}, \quad \Lambda_2 = \frac{\frac{1}{N} - \sigma_2}{\frac{1}{N} + \sigma_2}. \tag{11}$$

In addition, $\alpha_1^2 = 1$ for stochastic matrices and so for $\mathcal{H}$ when $\mathcal{H} = \mathcal{HD}$. Since the any deviation of the elements of the principal eigenvector from $\frac{1}{\sqrt{N}}$ would change the equality $\alpha_1^2 = 1$, we multiply variance by N to get total deviation from 1. Therefore, we define the estimate of α_1^2 as:

$$\tilde{\alpha}_1^{\,2} = \frac{(1 - N\sigma_1) + (1 - N\sigma_2)}{2}. \tag{12}$$

Note that $\tilde{\alpha}_1^{\,2}$ and $\tilde{P}_{reg_2}$ are only predictions and may fail to provide good estimates for particularly some structured matrices and matrices whose eigenvectors are close to the columns of an identity matrix. For instance, consider the following matrix:

$$\begin{pmatrix} 21.8214 & 0 & 0.6118 & 0.4983 \\ 0 & 14.2944 & 0.4983 & 0.6118 \\ 0.6118 & 0.4983 & 12.1626 & 0 \\ 0.4983 & 0.6118 & 0 & 5.4111 \end{pmatrix}. \tag{13}$$

The eigenvalues of this matrix are 5.3537, 12.0193, 14.4411, and 21.8753 respectively, associated with the following eigenvectors:

$$\begin{pmatrix} 0.0304613 & 0.0597207 & 0.0215934 & 0.9975166 \\ 0.0686662 & 0.2074209 & -0.9758165 & 0.0066086 \\ -0.0077623 & -0.9761393 & -0.2076080 & 0.0631720 \\ -0.9971443 & 0.0237068 & -0.0649217 & 0.0304360 \end{pmatrix}. \tag{14}$$

As computed from the above, the magnitudes of the sums of the components of the eigenvectors are very close to each other: $|-0.90578|, |-0.68529|, |-1.22675|$, and $|1.09773|$, respectively. In addition, the second eigenvector, not associated to the principal eigenvalue, has the largest sum.

Also, note that one can also predict α_1^2 from the distribution of the matrix elements. For instance,[21,24]

$$max_{ij} \frac{\mu_{1i}}{\mu_{1j}} \leq \frac{max_{ij} h_{ij}}{min_{ij} h_{ij}}, \tag{15}$$

where h_{ij}s are the non-zero matrix elements of $\mathcal{H}$. However, these bounds are generally not tight enough to give good estimates in many cases.

In Sec. 4, we shall show the comparisons of these estimates with the computed probabilities for random matrices.

3. Possible Applications

In the previous sections, we have showed that the positive eigenpair of an irreducible symmetric non-negative matrix can be obtained by using an initial equal superposition state when the estimated probabilities high. This eliminates the necessity of knowing an initial approximate eigenvector in the applications of the PEA to the problems involving non-negative matrices. Irreducible non-negative matrices are known to have positive eigenpairs due to Perron–Frobenious theorem. There is also more general but the same statements indicated in this theorem for compact operators.[25] One may also apply permutation matrices or splitting techniques to convert the interested matrix to a non-negative one or to increase the expected probability outcome when the probability is lower than an acceptable value.

Since a wide variety of problems in science can be represented by non-negative matrices, the PEA can be applied without an initial approximate eigenvector to these problems. In the following subsections, we shall consider two important classes among these problems: viz. the k-local Hamiltonian problem and the stochastic processes.

3.1. *Applications to local Hamiltonian problems*

One of the applications of the non-negative matrices can be found in quantum mechanics where such matrices are called stoquastic matrices[26,27] i.e. matrices with non-negative off-diagonal elements. If a Hamiltonian operator $\mathcal{H}$, a Hermitian operator acting on $(C^2)^{\otimes n}$, can be expressed as a sum of local Hamiltonians representing the interactions between at most k qubits, then it is called k-local n-qubit Hamiltonian. More formally, $\mathcal{H} = \sum_s H_s$. Finding the lowest eigenvalue of $\mathcal{H}$ defines an eigenvalue problem which is so-called local Hamiltonian problem. This eigenvalue problem can be also described as a decision problem to decide whether the ground state energy of $\mathcal{H}$ is at most a or at least b for given constants a and b such that $a \leq b$ and $b - a \leq 1/poly(n)$. This problem has been shown to be QMA-complete for $k \geq 2$[28] (for $k = 2$, it is QMA-complete only when both negative and positive signs in the Hamiltonian are allowed [29]).

For the local Hamiltonians with positive off-diagonal matrix elements in the standard basis, the matrix elements of the corresponding Gibbs density matrix, $\rho = e^{-\beta\mathcal{H}}/Tr(-\beta\mathcal{H})$, are all positive for any $\beta \geq 0$. Due to the theorem given above, the ground state energy of $\mathcal{H}$ with positive off-diagonal elements can be associated with the eigenvector whose coefficients are all positive. Because one can associate a probability distribution to the ground state, the nature of these Hamiltonians are considered similar to stochastic processes. Thus, the Hamiltonians of these types are called *stoquastic*.[26] (Note that the Hamiltonian is not a stochastic matrix whose rows and columns are sum to one and the principal eigenvalue is one associated with an eigenvector of all ones.)

3.2. *Applications to stochastic processes*

The PEA can find the principal eigenpair of a stochastic matrix with probability one[23] since the sum of the coefficients is one for the principal eigenvector and zero for the rest of the eigenvectors. However, the stochastic processes are generally defined by non-Hermitian matrices, which are also widely seen in quantum physics: the Hamiltonian of a closed system in equilibrium must be Hermitian to have real energy values. However, non-equilibrium processes and open systems connected to reservoirs can be only described by non-Hermitian models.[30]

3.2.1. *Simulation of non-Hermitian operators*

Any non-Hermitian matrix $\mathcal{H}$ can be decomposed into a Hermitian and a skew-Hermitian parts as:

$$\mathcal{H} = H + S = \frac{1}{2}(\mathcal{H} + \mathcal{H}^\dagger) + \frac{1}{2}(\mathcal{H} - \mathcal{H}^\dagger), \tag{16}$$

where $\mathcal{H}^\dagger$ describes the conjugate transpose of $\mathcal{H}$. Here, $H = \frac{1}{2}(\mathcal{H} + \mathcal{H}^\dagger)$ and $S = \frac{1}{2} \times (\mathcal{H} - \mathcal{H}^\dagger)$ define the nearest Hermitian and skew-Hermitian matrices to $\mathcal{H}$, respectively.[31] Therefore, the matrix H can be used as an approximation to $\mathcal{H}$ in the simulation.

A matrix $\mathcal{H}$ is called normal if $\mathcal{H}^\dagger\mathcal{H} - \mathcal{H}\mathcal{H}^\dagger = 0$. When $\mathcal{H}$ is a normal, it is easy to see that H and S also commute: $[H, S] = HS - HS = 0$. Moreover, because of the symmetry, all the eigenvalues of H are real and because of the skew symmetry, all the eigenvalues of S involve only imaginary parts. Since $\mathcal{H}\mathcal{H}^\dagger = \mathcal{H}^\dagger\mathcal{H}$, the eigenvectors of H and S are the same. In addition, the imaginary part of the eigenvalues of $\mathcal{H}$ are equal to the eigenvalues of S and the real parts are to the eigenvalues of H. Hence, using $U_1 = e^{iH}$ and $U_2 = e^S$ in the simulation, one can simulate the non-Hermitian operator $\mathcal{H}$ on quantum computers by using separate two registers to obtain the imaginary and the real parts of the eigenvalue. However, in the stochastic cases, if $\mathcal{H}$ is normal, it must be also doubly stochastic i.e. its left and right principal eigenvectors are already known to be a vector of all ones with the eigenvalue one. Therefore, instead of an approximate normal matrix, we can use the closest Hermitian matrix defined above as $H = \frac{1}{2}(\mathcal{H} + \mathcal{H}^\dagger)$.

In the non-stochastic cases, one can also try to instead find the closest normal matrix by following the Jacobi algorithm which attempts to diagonalize the matrix by using rotation matrices (Givens rotations) and converges to a matrix so-called ΔH. The best closest matrix in the Frobenius norm is then defined by the sum of the diagonal elements of ΔH and the rotation matrices used in the algorithm.[32,33] One can also procure a quantum circuit to implement this closest matrix by mapping rotation matrices to quantum gates as done in Ref. 34. However, since this algorithm is based on the eigenvalue decomposition, the eigenvalues (the diagonal elements of ΔH and the eigenvectors (the combination of the rotation matrices) are already generated for the found normal matrix.

4. Numerical Results

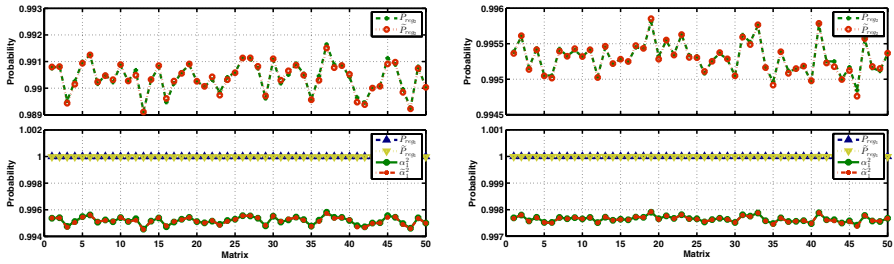
In this section, we compare the estimated probabilities $\tilde{\alpha}_1^2$, $\tilde{P}_{reg_1}$, and $\tilde{P}_{reg_2}$ with the computed probabilities α_1^2, P_{reg_1}, and P_{reg_2}, respectively, for the randomly generated matrices described as follows. In the simulations, we have used MATLAB and given sample code for the generation of random matrices. However, for the exploration of the quantum systems, it is much more efficient and easier to use one of the quantum tools provided by different research groups, e.g. QuTip [35,36] an open source toolbox quantum designed in Python.

4.1. *Random symmetric matrices with non-negative off-diagonal elements*

We generate a random symmetric matrix with non-negative off-diagonal elements as follows: first a random diagonal matrix and a strictly upper triangular sparse non-negative matrix are generated. Then, these matrices are combined to have a symmetric matrix with non-negative off-diagonal elements. This can be done in MATLAB as follows:

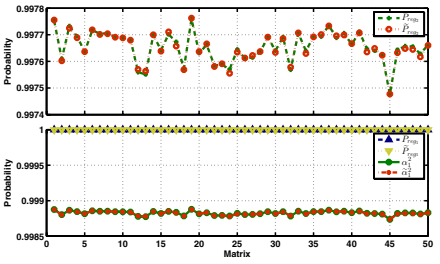
```
%MATLAB code to generate a random symmetric matrix
% with non-negative off-diagonal elements
R = triu(sprand(N,N,0.5),1); % N is the dimension,
% and 0.5 is the sparsity of the matrix.
L = randn(N,1);
H = R+R'+diag(L);
```

Figure 2 shows the comparisons of the estimated and computed probabilities for matrices of different dimensions generated by following the above code. As shown in the figure, the estimated and computed probabilities are almost the same and very high (close to one). Furthermore, the success probability, P_{reg_1}, with the Hadamard gates applied to $|reg_2\rangle$ in the end is almost one and higher than the probability, α_1^2, without the Hadamard gates.

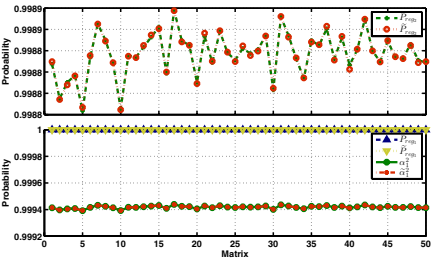


(a) 512 by 512 Matrices (b) 1,024 by 1,024 Matrices

Fig. 2. Representations of the comparisons of the estimated probabilities $\tilde{\alpha}_1^2$, $\tilde{P}_{reg_1} = \frac{\tilde{\alpha}_1^4}{\tilde{P}_{reg_2}}$, $\tilde{P}_{reg_2}$ with the computed probabilities α_1^2, $P_{reg_1} = \frac{\alpha_1^4}{P_{reg_2}}$, and P_{reg_2} for random non-negative symmetric matrices of different dimensions.



(c) 2,048 by 2,048 Matrices



(d) 4,096 by 4,096 Matrices

Fig. 2. (*Continued*)

4.2. *Random 3-local Hamiltonians*

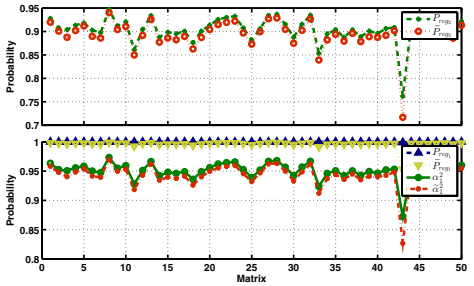
We employ the following Hamiltonian as the first example local Hamiltonian:

$$\mathcal{H}_{XZ} = \sum_{i,j,k} K_{ijk} X_i X_j X_k + J_{ijk} Z_i Z_j Z_k \tag{17}$$

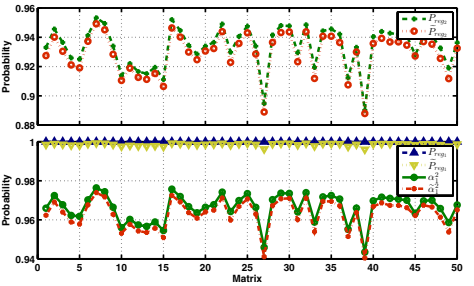
with $0 \leq K_{ijk} \leq 1$ and $-1 \leq J_{ijk} \leq 1$. Here, X and Z are the Pauli spin operators. Choosing K_{ijk} and J_{ijk} randomly, 50 numbers of random matrices are generated for each 9, 10, 11, 12, and 13 qubit systems and shows the estimated and computed probabilities in Fig. 3.

In the second example, one-body and two-body interaction terms are also included separately in the Hamiltonian:

$$\begin{aligned}\mathcal{H}_{XZ} = & \sum_i d_i X_i + h_i Z_i + \sum_{i,j} K_{1ij} X_i X_j + J_{1ij} Z_i Z_j \\ & + \sum_{i,j,k} K_{2ijk} X_i X_j X_k + J_{2ijk} Z_i Z_j Z_k\end{aligned} \tag{18}$$

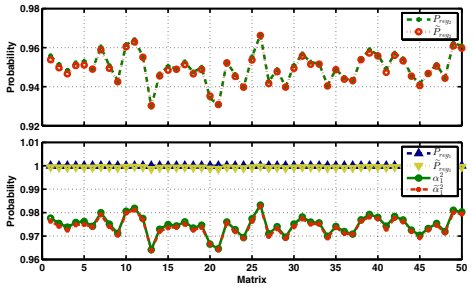


(a) 512 by 512 3-local Hamiltonians

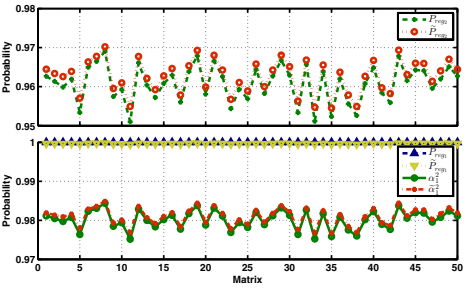


(b) 1,024 by 1,024 3-local Hamiltonians

Fig. 3. Representations of the comparisons of the estimated probabilities $\tilde{\alpha}_1^2$, $\tilde{P}_{reg_1} = \frac{\tilde{\alpha}_1^4}{\tilde{P}_{reg_2}}$, $\tilde{P}_{reg_2}$ with the computed probabilities α_1^2, $P_{reg_1} = \frac{\alpha_1^4}{P_{reg_2}}$, and P_{reg_2} for random 3-local Hamiltonians of different dimensions described in Eq. (17).



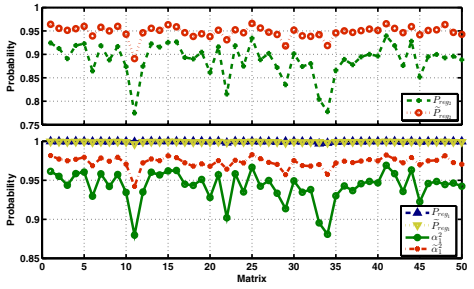
(c) 2,048 by 2,048 3-local Hamiltonians



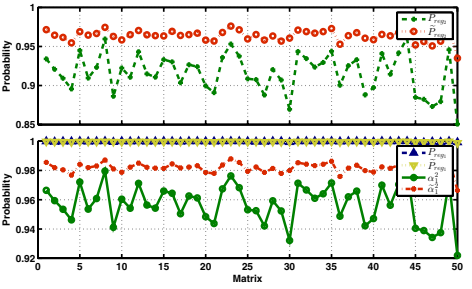
(d) 4,096 by 4,096 3-local Hamiltonians

Fig. 3. (*Continued*)

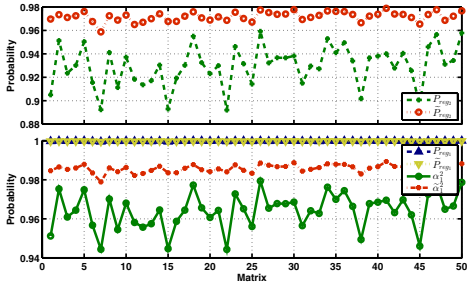
with $0 \leq d_i, K_{1ijk}, K_{2ijk} \leq 1$ and $-1 \leq h_i, J_{1ijk}, J_{2ijk} \leq 1$. As done in the first example, choosing the coefficients randomly, Hamiltonians of different sizes are generated. The results are shown in Fig. 4. As seen in the figure, the estimation is not as good as the cases in Figs. 2 and 3. This is because the ratio defined in Eq. (15) is



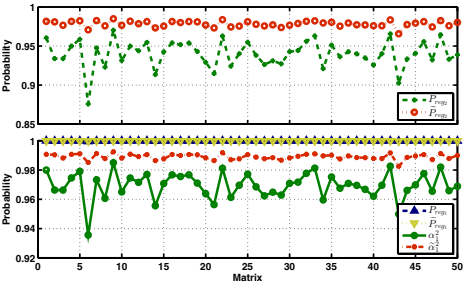
(a) 512 by 512 3-local Hamiltonians



(b) 1,024 by 1,024 3-local Hamiltonians



(c) 2,048 by 2,048 3-local Hamiltonians



(d) 4,096 by 4,096 3-local Hamiltonians

Fig. 4. Representations of the comparisons of the estimated probabilities $\tilde{\alpha}_1^{\,2}$, $\tilde{P}_{reg_1} = \frac{\tilde{\alpha}_1^{\,4}}{\tilde{P}_{reg_2}}$, $\tilde{P}_{reg_2}$ with the computed probabilities α_1^2, $P_{reg_1} = \frac{\alpha_1^4}{P_{reg_2}}$, and P_{reg_2} for random 3-local Hamiltonians of different dimensions described in Eq. (19).

generally higher for the matrices generated from Eq. (18) in comparison to the ones from Eq. (17).

5. Conclusion

In this paper, we have showed that the positive eigenpair of an irreducible symmetric non-negative matrix can be obtained when the estimated probabilities high. This eliminates the necessity of knowing an initial approximate eigenvector in the applications of the PEA to a wide variety of problems involving non-negative matrices. Here, we have also discussed how to apply it to local Hamiltonian problems and stochastic processes and showed the comparisons of the estimated success probabilities to the computed ones for random symmetric matrices and 3-local Hamiltonians.

Acknowledgment

This work is supported by TUBITAK under the grant number 115E774.

References

1. D. Deutsch, *Proc. Roy. Soc. London. A. Math. Phys. Sci.* **400** (1985) 97.
2. C. H. Bennett, E. Bernstein, G. Brassard and U. Vazirani, *SIAM J. Comput.* **26** (1997) 1510.
3. D. S. Abrams and S. Lloyd, *Phys. Rev. Lett.* **83** (1999) 5162.
4. A. Kitaev, *ECCC* **3** (1996).
5. L. F. Wei and F. Nori, *J. Phys. A Math. Gen.* **37** (2004) 4607.
6. H. Wang, L.-A. Wu, Y-xi. Liu and F. Nori, *Phys. Rev. A* **82** (2010) 062303.
7. A. Daskin and S. Kais, *J. Chem. Phys.* **134** (2011) 144112.
8. A. Daskin, A. Grama and S. Kais, *Quantum Inf. Process.* **13** (2014) 333.
9. A. Aspuru-Guzik, A. D. Dutoi, P. J. Love and M. Head-Gordon, *Sci.* **309** (2005) 1704.
10. I. Kassal, S. P. Jordan, P. J. Love, M. Mohseni and A. Aspuru-Guzik, *PNAS* **105** (2008) 18681.
11. H. Wang, S. Kais, A. Aspuru-Guzik and M. R. Hoffmann, *Phys. Chem. Chem. Phys.* **10** (2008) 5388.
12. L. Veis and J. Pittner, *J. Chem. Phys.* **133** (2010) 194106.
13. B. P. Lanyon, J. D. Whitfield, G. G. Gillett, M. E. Goggin, M. P. Almeida, I. Kassal, J. D. Biamonte, M. Mohseni, B. J. Powell, M. Barbieri, A. Aspuru-Guzik and A. G. White, *Nat. Chem.* **2** (2010) 106.
14. H. Wang, S. Ashhab and F. Nori, *Phys. Rev. A* **85** (2012) 062304.
15. D. Lu, B. Xu, N. Xu, Z. Li, H. Chen, X. Peng, R. Xu and J. Du, *Phys. Chem. Chem. Phys.* **14** (2012) 9411.
16. I. Kassal, J. D. Whitfield, A. Perdomo-Ortiz, H. Yung and A. Aspuru-Guzik, *Ann. Rev. Phys. Chem.* **62** (2011) 185.
17. I. M. Georgescu, S. Ashhab and F. Nori, *Rev. Mod. Phys.* **86** (2014) 153.
18. C. Meyer, *Matrix Analysis and Applied Linear Algebra Book and Solutions Manual*, Vol. 2 (Society for Industrial and Applied Mathematics, USA, 2000).
19. R. B. Bapat and T. ES. Raghavan, *Nonnegative Matrices and Applications*, Vol. 64 (Cambridge University Press, Cambridge, 1997).
20. A. Berman and R. J. Plemmons, *Math. Sci. Classics Appl. Math.* **9** (1979).

21. H. Minc, *SIAM J. Numer. Anal.* **7** (1970) 424.
22. I. Gutman, C. Rucker and G. Rucker, *J. Chem. Inf. Comput. Sci.* **41** (2001) 739.
23. A. Daskin, A. Grama and S. Kais, *Quantum Inf. Processing* **13** (2014) 2653.
24. S. M. Cioaba and D. A. Gregory, *Electron. J. Linear Al.* **16** (2007) 366.
25. Y. Du, Order structure and topological methods in nonlinear partial differential equations, *Krein-Rutman Theorem and the Principal Eigenvalue*, Vol. 2 (World Scientific, Singapore, 2006).
26. S. Bravyi, D. P. Divincenzo, R. Oliveira and B. M. Terhal, *Quantum Inf. Comput.* **8** (2008) 361.
27. S. Bravyi and B. Terhal, *SIAM J. Comput.* **39** (2010) 1462.
28. J. Kempe, A. Kitaev and O. Regev, *SIAM J. Comput.* **35** (2006) 1070.
29. S. P. Jordan, D. Gosset and P. J. Love, *Phys. Rev. A* **81** (2010) 032331.
30. K. B. Efetov, *Phys. Rev. Lett.* **79** (1997) 491.
31. J. B. Keller, *Math. Magazine* **48** (1975) 192.
32. N. J. Higham, Matrix nearness problems and applications, in *Applications of Matrix Theory* (Oxford University Press, Oxford 1989), pp. 1–27.
33. Axel Ruhe, Closest normal matrix finally found! BIT *Numer. Math.* **27** (1987) 585.
34. J. J. Vartiainen, M. Möttönen and M. M. Salomaa, *Phys. Rev. Lett.* **92** (2004) 177902.
35. J. R. Johansson, P. D. Nation and F. Nori, *Comput. Phys. Commun.* **183** (2012) 1760.
36. J. R. Johansson, P. D. Nation and F. Nori, *Comput. Phys. Commun.* **184** (2013) 1234.