Quantum polar decomposition algorithm

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Abstract: The polar decomposition for a matrix $A$ is $A = UB$, where $B$ is a positive Hermitian matrix and $U$ is unitary (or, if $A$ is not square, an isometry). This paper shows that the ability to apply a Hamiltonian $\begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}$ translates into the ability to perform the transformations $e^{-iBt}$ and $U$ in a deterministic fashion. We show how to use the quantum polar decomposition algorithm to solve the quantum Procrustes problem, to perform pretty good measurements, to find the positive Hamiltonian closest to any Hamiltonian, and to perform a Hamiltonian version of the quantum singular value transformation.

The polar decomposition of a matrix is $A = UB = \tilde{B}U$, where $B = (A^\dagger A)^{1/2}$, $\tilde{B} = (AA^\dagger)^{1/2}$ are positive Hermitian matrices, and $U = A(A^\dagger A)^{-1/2} = (AA^\dagger)^{-1/2}A$ is unitary (when $A$ is square) or an isometry (when $A$ is not square). The polar decomposition has many applications in linear algebra [1-2]. $U$ is in essence the ‘closest’ unitary to $A$: it is the unitary that minimizes $\|U - A\|_2$ in Frobenius norm. In a quantum mechanical setting, it would be useful to have a method which allows one to perform the polar decomposition. This paper generalizes the quantum linear systems algorithm [3-4] to construct just such a quantum algorithm for the polar decomposition. In particular, given the ability to apply a Hamiltonian $H = \begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}$, we show how to apply the unitary/isometry $U$ in
time $O(\kappa)$, where $\kappa$ is the condition number of $A$, and how to apply the transformations $e^{-iBt}$, $e^{-i\tilde{B}t}$ in time $O(\kappa t/\epsilon)$, where $\epsilon$ is the accuracy to which these transformations are to be performed. The time taken to perform the quantum polar decomposition is independent of the dimension of the Hilbert space on which $H$ acts: for example $A$ could be an operator acting on the infinite dimensional Hilbert space for a collection of modes of the electromagnetic field.

We apply the algorithm to reconstruct unitary transformations from examples of input-output pairs – the quantum Procrustes problem [2], to perform pretty good measurements, and to find the positive matrix closest to any Hermitian matrix [1]. In its generalized form, the quantum polar decomposition algorithm can be considered to be a Hamiltonian version of the quantum singular value decomposition [5].

Preliminaries

Write the $m \times n$ matrix $A$ as $A = \sum_j \sigma_j \ell_j r_j^\dagger$, where $\sigma_j$ are the singular values of $A$ and $\ell_j \in \mathcal{H}_L = C^m$, $r_j \in \mathcal{H}_R = C^n$ are the corresponding left and right singular vectors. The polar decomposition matrices are then $U = \sum_j \ell_j r_j^\dagger$, an isometry from $\mathcal{H}_R$ to $\mathcal{H}_L$, $B = \sum_j \sigma_j r_j r_j^\dagger$, acting on $\mathcal{H}_R$, and $\tilde{B} = \sum_j \sigma_j \ell_j \ell_j^\dagger$, acting on $\mathcal{H}_L$. Suppose that one has the ability to apply a Hamiltonian $\pm H$, where $H = A + A^\dagger$ acts on the Hilbert space $\mathcal{H}_R \oplus \mathcal{H}_L$. $H = A + A^\dagger$ can also be represented in matrix form as

$$H = \begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}. \tag{1}$$

We show how to use the ability to apply the Hamiltonian $\pm H$ to perform the transformations $e^{-iBt}$, $e^{-i\tilde{B}t}$ and $U$, in a deterministic fashion. While we will present the quantum polar transformation in terms of matrices, we also show that the entire construction of the quantum polar decomposition goes through when $A$ is an operator on an infinite dimensional space, e.g., a polynomial in annihilation and creation operators on a set of harmonic oscillators.

Generalized quantum linear systems algorithm

The quantum polar decomposition algorithm is based on a deterministic extension of the original non-deterministic quantum linear systems algorithm [3]. The generalized version of the original quantum linear systems algorithm operates as follows. For a generic
Hermitian $H$ with eigenvectors $|j\rangle$ and eigenvalues $\lambda_j$, we first review how to perform the transformation

$$|\psi\rangle \rightarrow e^{-if(H)}|\psi\rangle = \sum_j e^{-if(\lambda_j)}\psi(j)|j\rangle,$$

(2)

where $|\psi\rangle = \sum_j \psi(j)|j\rangle$. Here $f$ can be any computable function of the eigenvalues. To accomplish the transformation in equation (2), we employ the quantum phase estimation algorithm [6] – a digitized version of the von Neumann pointer variable model of measurement [7] – to correlate the eigenvectors of $H$ with estimates of the corresponding eigenvalues:

$$|\psi\rangle \otimes |x = 0\rangle \rightarrow \sum_j \psi(j)|j\rangle \otimes |\tilde{\lambda}_j\rangle,$$

(3)

where $\tilde{\lambda}_j$ is a $b$-bit approximation to $\lambda_j$. Now multiply each term by a phase that is a function of the estimated eigenvalue to obtain

$$\sum_j \psi(j)e^{-if(\tilde{\lambda}_j)}|j\rangle \otimes |\tilde{\lambda}_j\rangle.$$

(4)

Undoing the quantum phase estimation algorithm yields the desired transformation of equation (2) to $b$ bits of accuracy in $\lambda_j$.

To perform the transformation (2) in infinite dimensional systems, adjoin a continuous variable with position/momentum operators $X,P$: $[X,P] = i$. Perform von Neumann’s Hamiltonian pointer variable model of measurement [7]: apply the Hamiltonian $H \otimes P$ to the initial state $|\psi\rangle \otimes |x = 0\rangle$ for a unit time interval $t = 1$ to create the state $\sum_j \psi_j|j\rangle \otimes |\lambda_j\rangle$, the continuous variable version of equation (3). Now use methods of continuous variable quantum computation [8] to apply the Hamiltonian $f(X)$ to the pointer variable, again for unit time, yielding the state $\sum_j \psi_j e^{-if(\lambda_j)}|j\rangle \otimes |\lambda_j\rangle$. If $f$ is a $q$th order polynomial in $X$ this step takes time $O(q)$. Finally, apply the Hamiltonian $-H \otimes P$ for unit time. The result is the state

$$e^{iH \otimes P}(I \otimes e^{-if(X)})e^{-iH \otimes P}|\psi\rangle \otimes |x = 0\rangle = e^{-if(H)}|\psi\rangle \otimes |x = 0\rangle,$$

(5)

which is again the desired transformation of equation (2), but now in the context of infinite-dimensional operators rather than finite-dimensional matrices.
Quantum polar transformation algorithm

Framed in the background of the generalized linear systems algorithm, the quantum polar transformation immediately reveals itself. To perform the polar transformation unitary/isometry \( U \), take \( f(x) = (\pi/2)(1 - \text{sign}(x)) \) in equation (2). This transformation multiplies an eigenvector of \( H \) by the sign of its eigenvalue. The eigenvectors of \( H \) take the form

\[
\begin{pmatrix}
0 & A^+ \\
A & 0
\end{pmatrix}
\begin{pmatrix}
r_j \\
\pm \ell_j
\end{pmatrix} = \pm \sigma_j
\begin{pmatrix}
r_j \\
\pm \ell_j
\end{pmatrix}.
\]

Using the relationships given above between the eigenvectors and eigenvalues of \( H \) with the left and right singular vectors and the singular values of \( A \), we see that

\[
\begin{pmatrix}
r_j \\
0
\end{pmatrix} = (1/2) \left( \begin{pmatrix}
r_j \\
\ell_j
\end{pmatrix} + \begin{pmatrix}
r_j \\
-\ell_j
\end{pmatrix} \right) \rightarrow (1/2) \left( \begin{pmatrix}
r_j \\
\ell_j
\end{pmatrix} - \begin{pmatrix}
r_j \\
-\ell_j
\end{pmatrix} \right) = \begin{pmatrix}
0 \\
\ell_j
\end{pmatrix}.
\]

Similarly,

\[
\begin{pmatrix}
0 \\
\ell_j
\end{pmatrix} \rightarrow \begin{pmatrix}
r_j \\
0
\end{pmatrix}.
\]

Writing the outcome of the transformation in both matrix and quantum bra-ket notation, we see that the outcome of the generalized quantum linear systems algorithm is the state

\[
\left( \sum_j |\ell_j\rangle\langle r_j| + \sum_j |r_j\rangle\langle \ell_j| \right) \psi = (U + U^\dagger)\psi = \begin{pmatrix}
0 & U^\dagger \\
U & 0
\end{pmatrix} \left( \begin{pmatrix} |\psi\rangle_R \\
|\psi\rangle_L \end{pmatrix} \right).
\]

Thus, as promised, we can perform the unitary/isometry \( U \) on \( H_R \), and \( U^\dagger \) on \( H_L \), where \( U \) is the unitary/isometry in the polar decomposition of \( A \).

Without loss of generality, take the largest singular value of \( A \) to be one. The condition number of \( A \) is then the inverse of the smallest singular value \( \kappa = \sigma_{\min}^{-1} \). To perform the quantum phase estimation algorithm sufficiently accurately to resolve the sign of the smallest eigenvalue then takes time \( O(\kappa) \).

Following reference [3], we can also perform \( U \) only on the well-conditioned subspace of \( A \). When the quantum phase algorithm yields an estimate of the singular value that is smaller than some value \( 1/\bar{\kappa} \), we decline to change its sign, and flip a ‘flag’ qubit, initially in the state \( |0\rangle \), to the value \( |1\rangle \). This procedure allows us to project onto the well-conditioned subspace spanned by singular vectors whose singular value is greater than or equal to the inverse of the chosen effective condition number \( \bar{\kappa} \), and to perform \( U \) only on this subspace. The operation performs

\[
U_{\bar{\kappa}} + U_{\bar{\kappa}}^\dagger = \sum_{j: \sigma_j \geq 1/\bar{\kappa}} |\ell_j\rangle\langle r_j| + |r_j\rangle\langle \ell_j|
\]
on the well-conditioned subspace, and the identity on the poorly conditioned subspace, raising a flag if the operation has projected the initial state on the poorly conditioned subspace. The algorithm takes time \(O(\tilde{\kappa})\).

Now take \(f(x) = |x|t\) in the quantum phase estimation algorithm. The resulting transformation is

\[
(e^{-i\sqrt{A^\dagger A}t} + e^{-i\sqrt{AA^\dagger}t})\psi.
\] (11)

To perform this transformation to accuracy \(\epsilon\) takes time \(O(\kappa t/\epsilon)\). So we can perform the transformations \(e^{-iBt}\) on \(H_R\) and \(e^{-i\tilde{B}t}\) on \(H_L\) as well. QED = Quod Erat Demonstrandum = Quite Easily Done.

**Generalization**

Writing \(f(A) = \sum_j f(\sigma_j)|\ell_j\rangle\langle r_j|\), the same methods allow us to apply any Hamiltonian of the form

\[
f(A) + f(A)^\dagger, \quad f(\sqrt{A^\dagger A}) + f(\sqrt{AA^\dagger}).
\] (12)

In addition, we can apply any Hamiltonian of the form \(f(K) + f(K^\dagger)\), where \(K, K^\dagger\) have the same eigenvectors as \(\sqrt{A^\dagger A}, \sqrt{AA^\dagger}\), and the same eigenvalues up to a sign \(\pm 1\).

**Applications**

The polar decomposition is widely applicable for problems where we wish to find the closest matrix of a particular form to a given matrix [1]. When \(A\) is Hermitian, then \(B = \tilde{B}\) is the closest positive Hermitian matrix to \(A\) in Frobenius norm. Similarly, \(U\) is the solution to the problem of minimizing \(\|U - A\|_2\) over all unitaries/isometries. We now apply the quantum polar decomposition to the problem of finding and applying a unitary transformation given examples of input/output pairs, and to performing pretty good measurements. We show that the polar decomposition algorithm can be thought of as a Hamiltonian version of the quantum singular value transformation.

**Recreating a unitary from input/output pairs**

Suppose that we are given \(r\) input/output pairs

\[
\{(|\phi_j\rangle, |\psi_j\rangle)\} \in \mathcal{H}_0 \oplus \mathcal{H}_1.
\] (13)
Assume that we can coherently apply the transformations
\[ |j⟩ \otimes |0⟩ \rightarrow |j⟩ \otimes |φ_j⟩, \quad |j⟩ \otimes |0⟩ \rightarrow |j⟩ \otimes |ψ_j⟩, \] (14)
where \( |j⟩ \) are computational basis states. We wish to find the unitary/isometry \( U \) that minimizes
\[ \|UF − G\|^2, \] (15)
where \( F \) is the matrix whose columns are the \( \{|φ_j⟩\} \), and \( G \) is the matrix whose columns are the \( \{|ψ_j⟩\} \). This is the quantum Procrustes problem [2]. (Procrustes was a mythical bandit in ancient Greece, who would compare anyone he captured to the size of his bed, and then either stretch out or chop off the parts he needed to make the captive fit. Here, we are trying to fit \( F \) as non-violently as possible to \( G \) by a unitary/orthogonal transformation.)

To minimize the distance of \( U \) from the desired transformation, equation (15), subject to the constraint that \( U \) is a unitary/isometry, define a Lagrangian
\[ L = \sum_{j=1}^{r} \| |ψ_j⟩ − U |φ_j⟩ \|^2 − \text{tr}Λ(UU^† − I), \] (16)
where \( Λ \) is a positive Hermitian matrix of Lagrange multipliers. Taking the variation of \( L \) with respect to \( U \) and to \( Λ \), we find that the extremum is attained for \( U = A(A^†A)^{-1/2}, \) where \( A = \sum_{j=1}^{r} |ψ_j⟩⟨φ_j|. \) That is, the solution to the Procrustes problem is the unitary \( U \) of the polar decomposition of the matrix \( A \) relating inputs to outputs.

Note that unitaries of the form \( U = A\widetilde{K} \), where \( \widetilde{K} \) has the same eigenvectors as \((A^†A)^{-1/2} \) and the same eigenvalues up to a sign \( ±1 \), are also solutions to the Lagrange equations. Direct substitution into equation (15) shows that \( \widetilde{K} = (A^†A)^{-1/2} \) gives the unitary/isometry with minimum distance to \( A \), with the other solutions corresponding to local maxima. The global maximum (reverse Procrustes problem [2]) occurs when all the eigenvalues are negative: \( −U \) maximizes the distance in equation (15).

To apply the Hamiltonian \( H = A + A^† \) we use our quantum access to the input output pairs to create the state
\[ \frac{1}{\sqrt{2r}} \sum_{j=1}^{r} |j⟩ \otimes \left( |φ_j⟩|ψ_j⟩ \right). \] (17)
Tracing out the first register, we find the second register is in the state given by the density matrix
\[ ρ_A = \frac{1}{2r} \begin{pmatrix} C & A^† \\ A & Ĉ \end{pmatrix}, \] (18)
where \( C = (1/2r) \sum_j |\phi_j\rangle\langle\phi_j| \) and \( \tilde{C} = (1/2r) \sum_j |\psi_j\rangle\langle\psi_j| \). Let \( P_0, P_1 \) be the projectors onto \( \mathcal{H}_0, \mathcal{H}_1 \) respectively, By applying the unitary transformation \( V = P_0 - P_1 \), we can also create the state,

\[
\tilde{\rho}_A = V \rho_A V^\dagger = \frac{1}{2r} \begin{pmatrix} C & -A^\dagger \\ -A & \tilde{C} \end{pmatrix}.
\]

(19)

Now we use density matrix exponentiation [9] to apply the infinitesimal transformation

\[
e^{i\Delta t \tilde{\rho}_A} e^{-i\Delta t \rho_A} = I + i\Delta t \tilde{\rho}_A - i\Delta t \rho_A + O(\Delta t^2)
\]

\[
= I - i\Delta t(A + A^\dagger)/r + O(\Delta t^2) = e^{-i\Delta t(A+A^\dagger)/r} + O(\Delta t^2).
\]

(20)

That is, we can effectively apply the Hamiltonian \( H = A + A^\dagger \), and so can apply the quantum Procrustes transformation \( U \) on any state \( |\chi\rangle \) via the quantum polar decomposition algorithm. The algorithm takes time \( O(r\kappa) \), where \( r \) is the number of input-output pairs and \( \kappa \) is the condition number of \( A = \sum_{j=1}^r |\psi_j\rangle\langle\phi_j| \). An even more general solution to the quantum Procrustes problem is provided by the quantum emulation algorithm [10], which does not require the assumption that we can access the input-output state pairs in quantum superposition.

**Hamiltonian quantum singular value transformation**

The method used in the previous section shows how to perform a Hamiltonian version of the quantum singular value transformation [5]. Let \( A \) be any \( m \times n \) off-diagonal block of a Hamiltonian that we are able to apply. As we are only interested in the time evolution on the subspace acted on by \( A \) and \( A^\dagger \), without loss of generality we can simply consider Hamiltonians acting on \( \mathcal{H}_0 \oplus \mathcal{H}_1 \) of the form \( \pm M \), where

\[
M = \begin{pmatrix} D & A^\dagger \\ A & \tilde{D} \end{pmatrix},
\]

(21)

where \( D, \tilde{D} \) are arbitrary Hermitian matrices. Now use the same trick as above: apply \( M \) for time \( \Delta t \), followed by the unitary transformation \( V = P_0 - P_1 \), where \( P_0, P_1 \) are the projectors onto \( \mathcal{H}_0, \mathcal{H}_1 \). The resulting transformation is equivalent to the application of a Hamiltonian

\[
VMV^\dagger = \begin{pmatrix} D & -A^\dagger \\ -A & \tilde{D} \end{pmatrix}.
\]

(22)

By the first order Trotterization trick of equation (19) above, and noting that we can apply \( \pm M \) and so also \( \pm VMV^\dagger \), we can then apply the effective Hamiltonian

\[
(M - VMV^\dagger)/2 = \begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}.
\]

(23)
The ability to apply this Hamiltonian then translates into the ability to apply any Hamiltonian with the same singular vectors as $A$, and whose singular values are some computable function of the singular values of $A$ as in equation (12) above. The Hamiltonian singular value transformation can be extended to infinite dimensional systems via the techniques of equation (5) above. It is an open question whether it is possible to use the methods of references [4-5] to forego the use of the quantum phase estimation algorithm and to apply such Hamiltonians more efficiently.

**Pretty good measurements**

Suppose that we wish to enact the pretty good (square root) measurement to distinguish between $n$ states $\{|\phi_j\rangle\}$. The pretty good measurement for distinguishing between pure states consists of projections onto the states

$$|\chi_j\rangle = \left(\sum_j |\phi_j\rangle\langle\phi_j|\right)^{-1/2} |\phi_j\rangle.$$  \hspace{1cm} (24)

That is, as shown in [11], the pretty good measurement is simply a von Neumann measurement that projects onto the rows of $U = A(A^\dagger A)^{-1/2}$, where $A = \sum_j |j\rangle\langle\phi_j|$ is the matrix whose rows are $\{|\phi_j\rangle\}$.

This measurement can be performed efficiently using the quantum polar decomposition algorithm. In the algorithm from the previous section for performing the polar decomposition unitary $U$ given quantum access to the input output pairs $\{(|\phi_j\rangle, |\psi_j\rangle)\}$, take $|\psi_j\rangle = |j\rangle$. To perform the pretty good measurement on a state with density matrix $\rho$, first perform the unitary $U$ then measure in the $|j\rangle$ basis. The result $|j\rangle$ occurs with probability

$$p(j) = \langle j|U\rho U^\dagger|j\rangle = \langle j|A(A^\dagger A)^{-1/2}\rho(A^\dagger A)^{-1/2}A^\dagger|j\rangle = \langle \chi_j|\rho|\chi_j\rangle,$$  \hspace{1cm} (25)

which from equation (24) are just the probabilities for the pretty good measurement. To re-prepare the output state $|\chi_j\rangle$ – that is, to leave the system in the eigenstate of the pretty good measurement – then simply apply the unitary $U^\dagger$ to the state $|j\rangle$.

**Conclusion:** The polar decomposition of a matrix $A$ is $A = UB = \tilde{B}U$, where $U = A(A^\dagger A)^{-1/2}$ is unitary, and $B = (A^\dagger A)^{1/2}$, $\tilde{B} = (AA^\dagger)^{1/2}$ are positive Hermitian matrices.
This paper showed how the ability to apply the Hamiltonian $\begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}$ translates into the ability to perform $e^{-iBt}$, $e^{-i\tilde{B}t}$ and $U$ in a deterministic fashion. The algorithm is based on the original linear systems algorithm [3] and takes time $O(\kappa)$ to perform $U$, where $\kappa$ is the condition number of $A$. The time taken to perform the algorithm is independent of the dimension of the Hilbert space. Indeed, the Hamiltonian $H$ could act on an infinite dimensional Hilbert space, corresponding, e.g., to modes of the electromagnetic field.

The polar decomposition has many potential applications in linear algebraic protocols [1-2]. Here, we showed how to use the quantum polar decomposition algorithm to perform the optimal unitary that approximately reproduces a set of input/output pairs (the quantum Procrustes problem), to apply the positive Hamiltonian that is closest to a given Hamiltonian, and to perform pretty good measurements corresponding to a set of pure states. The method employed can be thought of as a Hamiltonian version of the quantum singular value transformation [5].

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