Lecture 3: Operators in quantum computing

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We saw that the states of a quantum system can be described as a vector. We also looked at linear operators on these vectors. This lecture will extend our understanding of these linear operators and mention postulate which specifies the operators allowed in quantum computing.

1 Eigenvalues and eigenvectors

A matrix $M \in L(V, W)$ is square if $dim(V) = dim(W)$. In particular, a matrix $M \in L(V)$ is always square. For a matrix $M \in L(V)$, a vector $v \in V$ satisfying,

$$Mv = \lambda v \text{ for some } \lambda \in \mathbb{C},$$

is called the *eigenvector* of matrix M with *eigenvalue* λ.

Exercise 1. Given two eigenvectors v, w, when is their linear combination an eigenvector itself?

The previous exercise can be used to show that all the eigenvectors corresponding to a particular eigenvalue form a subspace. This subspace is called the *eigenspace* of the corresponding eigenvalue.

An eigenvalue λ of an $n \times n$ matrix M satisfies the equation

$$Det(\lambda I - M) = 0,$$

where $Det(M)$ denotes the determinant of the matrix M. The polynomial $Det(\lambda I - M) = 0$, in λ, is called the *characteristic polynomial* of M. The characteristic polynomial has degree n and will have n roots in the field of complex numbers. Though, these roots might not be real.

Exercise 2. Give an example of a matrix with no real eigenvalue.

The next theorem shows that the eigenvalues are preserved under the action of a full rank matrix.

Theorem 1. *Given a matrix P of full rank, matrix M and matrix $P^{-1}MP$ have the same set of eigenvalues.*

Proof. Suppose λ is an eigenvalue of $P^{-1}MP$, we need to show that it is an eigenvalue for M too. Say λ is an eigenvalue with eigenvector v. Then,

$$P^{-1}MPv = \lambda v \Rightarrow M(Pv) = \lambda Pv.$$

Hence Pv is an eigenvector with eigenvalue λ.

The opposite direction follows similarly. Given an eigenvector v of M, it can be shown that $P^{-1}v$ is an eigenvector of $P^{-1}MP$.

$$P^{-1}MP(P^{-1}v) = P^{-1}Mv = \lambda P^{-1}v$$

Hence proved. $\square$

Exercise 3. Where did we use the fact that P is a full rank matrix?

1.1 Spectral decomposition

Let us fix vector space V to be $\mathbb{C}^n$ going forward.

Exercise 4. Let v_1, v_2 be two eigenvectors of a matrix M with distinct eigenvalues. Show that these two eigenvectors are linearly independent.

Given an $n \times n$ matrix M, it need not have n linearly independent eigenvectors. Can it have more than n linearly independent eigenvectors? The matrix M is called *diagonalizable* iff the set of eigenvectors of M span the complete space $\mathbb{C}^n$. Let P be the matrix whose columns are n linearly independent eigenvectors, then $P^{-1}MP$ will be a diagonal matrix. By Theorem 1, our original matrix and this diagonal matrix will have same eigenvalues.

Exercise 5. What are the eigenvalues and eigenvectors of a diagonal matrix?

For a diagonalizable matrix, the basis of eigenvectors need not be an orthonormal basis. We will show a characterization of matrices whose eigenvectors can form an orthonormal basis. Fortunately, these matrices are of great importance in quantum computing, and are called *normal* matrices.

A *normal* matrix is defined to be a matrix M, s.t., $MM^* = M^*M$. Spectral theorem shows that we can form an orthonormal basis of $\mathbb{C}^n$ using the eigenvectors of a normal matrix.

Theorem 2 (Spectral theorem). *For a normal matrix $M \in L(\mathbb{C}^k)$, there exists an orthonormal basis $\{|x_1\rangle, \cdots, |x_k\rangle\}$ of $\mathbb{C}^k$ and $\lambda_i \in \mathbb{C}$ $(\forall i \in [k])$ such that*

$$M = \sum_{i=1}^{n} \lambda_i |x_i\rangle\langle x_i|.$$

Note 1. It means that any normal matrix $M = U^*DU$ for a diagonal matrix D with entries λ_i and the matrix U with $|x_i\rangle$ as columns.

Exercise 6. Show that $|x_i\rangle$ is an eigenvector of M with eigenvalue λ_i.

Note 2. $\langle y|x\rangle$ is a scalar, but $|y\rangle\langle x|$ is a matrix.

Note 3. The λ_i's need not be different. If we collect all the $|x_i\rangle$'s corresponding to a particular eigenvalue λ, the space spanned by those $|x_i\rangle$'s is the eigenspace of λ.

Proof idea. The proof of spectral theorem essentially hinges on the following lemma.

Lemma 1. *Given an eigenspace S (of eigenvalue λ) for a normal matrix M, then M acts on the space S and $S^\perp$ separately. In other words, $M|v\rangle \in S$ if $|v\rangle \in S$ and $M|v\rangle \in S^\perp$ if $|v\rangle \in S^\perp$.*

Proof of lemma. Since S is an eigenspace, $M|v\rangle \in S$ if $|v\rangle \in S$. For a vector $|v\rangle \in S$,

$$MM^*|v\rangle = M^*M|v\rangle = \lambda M^*|v\rangle.$$

This shows that M^* preserves the subspace S. Suppose $|v_1\rangle \in S^\perp$ and $|v_2\rangle \in S$, then $M^*|v_2\rangle \in S$. So,

$$0 = \langle v_1|M^*|v_2\rangle = \langle Mv_1|v_2\rangle.$$

Above equation implies $M|v_1\rangle \in S^\perp$. Hence, matrix M acts separately on S and $S^\perp$. □

The lemma implies that M is a linear operator on $S^\perp$, i.e., it moves every element of $S^\perp$ to an element in $S^\perp$ linearly. It can be easily shown that this linear operator (the action of M on $S^\perp$) is also normal. The proof of spectral theorem follows by using induction and is given below.

From the fundamental theorem of Algebra, there is at least one root λ_0 of $det(\lambda I - M) = 0$. Start with the eigenspace of the eigenvalue λ_0. Using Lem. 1, we can restrict the matrix to orthogonal subspace (which is of smaller dimension). We can divide the entire space into orthogonal eigenspaces by induction.

Exercise 7. Show that if we take the orthonormal basis of all these eigenspaces, then we get the required decomposition.

Exercise 8. Given the spectral decomposition of M, what is the spectral decomposition of M^*?

$\square$

Exercise 9. If M is normal, prove that the rank of M is the sum of the dimension of the non-zero eigenspaces.

It is easy to show that any matrix with orthonormal set of eigenvectors is a normal matrix. Hence, spectral decomposition provides another characterization of normal matrices.

Clearly the spectral decomposition is not unique (essentially because of the multiplicity of eigenvalues). But the eigenspaces corresponding to each eigenvalue are fixed. So there is a unique decomposition in terms of eigenspaces and then any orthonormal basis of these eigenspaces can be chosen.

Note 4. It is also true that if an eigenvalue is a root of characteristic polynomial with multiplicity k, then its eigenspace is of dimension k.

Spectral decomposition allows us to define functions over normal matrices.

Operator functions: Suppose we have a function, $f : \mathbb{C} \to \mathbb{C}$, from complex numbers to complex numbers. It can naturally extended to be a function on a normal linear operator in $L(\mathbb{C}^n)$. By definition of operator function, we apply the function on all the eigenvalues of the operator. So, if

$$A = \lambda_1 x_1 x_1^* + \cdots + \lambda_n x_n x_n^*.$$

then

$$f(A) = f(\lambda_1) x_1 x_1^* + \cdots + f(\lambda_n) x_n x_n^*.$$

In particular, we can now define the square-root, exponential and logarithm of an operator.

Note 5. This means that we define square root only for positive semi-definite operators.

Pauli matrices are used widely in quantum computing. They are defined as,

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

X is the quantum NOT gate and Z is known as the phase gate.

Exercise 10. Show that the Pauli matrices are Hermitian as well as Unitary by calculating their eigenvalue.

Exercise 11. Show that the Pauli matrices (with identity) form a basis of all Hermitian 2×2 operators.

Exercise 12. Find e^{iX}, e^{iY}, e^{iZ}.

Trace: Another very important function on operators introduced before is *trace*. We defined trace to be $Tr(A) = \sum_i A_{ii}$. At this point, it is a function on matrices and not linear operators.

Exercise 13. What is the problem?

For a linear operator, trace might be different for different bases. In other words, there is no guarantee that it is independent of the basis (from the definition given above).

Exercise 14. Show that the trace is cyclic, i.e., $tr(AB) = tr(BA)$.

This exercise implies that $tr(U^* A U) = tr(A)$. Hence, trace is independent of the representation.

Exercise 15. Show that $tr(|u\rangle\langle v|) = \langle u|v\rangle$.

If $M = \sum_{i=1}^{n} \lambda_i |x_i\rangle\langle x_i|$, the previous exercise shows that $tr(M) = \sum_i \lambda_i$. Since λ_i's do not depend on the basis chosen, this gives us a basis independent definition of trace. This definition allows us to define trace of a linear operator (and not just a matrix).

We also know that $\langle v|A|w\rangle = \sum_{ij} A_{ij} v_i^* w_j$.

Exercise 16. Show that $A_{ij} = \langle i|A|j\rangle$, where matrix A is represented in the standard basis $|1\rangle, \cdots, |n\rangle$.

From the previous exercise, $tr(A) = \sum_i \langle i|A|i\rangle$. In fact, for any orthonormal basis $v_1, \cdots, v_n$,

$$tr(A) = \sum_i \langle v_i|A|v_i\rangle,$$

(trace is indepedent of the basis.

If we take v_i to be the eigenvectors, we get the same equation

$$tr(A) = \sum_i \lambda_i.$$

Here, λ_i are the eigenvalues of the operator A.

2 Special class of matrices

We know that all eigenvalues of a normal matrix are complex numbers. We can pick any set of complex numbers and an orthonormal basis, that will give us a normal matrix. Why?

If we impose more constraints on the eigenvalues, it give us specific classes of normal matrices, very important for quantum computing. Before we take a look at these special classes of normal matrices, look at this useful notation again.

Given a square $n \times n$ matrix M and two vectors $u, v \in \mathbb{C}^n$,

$$\langle u|M|v\rangle := u^* M v = \langle u|Mv\rangle = \langle M^* u|v\rangle.$$

Exercise 17. Show that $\langle u|M|v\rangle = M \bullet |u\rangle\langle v|$.

Exercise 18. Let spectral decomposition of M be $\sum_i \lambda_i |x_i\rangle\langle x_i|$ and $v = \sum_i \alpha_i |x_i\rangle$. Find $\langle u|M|v\rangle$ in terms of λ_i, x_i, α_i.

2.1 Hermitian matrix

A matrix M is said to be *Hermitian* if $M = M^*$. It is easy to check that any Hermitian matrix is normal. You can also show that all the eigenvalues of a Hermitian matrix are real (given as an exercise).

Conversely if all the eigenvalues are real for a normal matrix then the matrix is Hermitian (from spectral theorem).

Note 6. In quantum meachanics, we use eigenvalues to denote the physical properties of a system. Since these quantities should be real, we use Hermitian operators.

For any matrix B, a matrix of the form B^*B or $B + B^*$ is always Hermitian. The sum of two Hermitian matrices is Hermitian, but the multiplication of two Hermitian matrices need not be Hermitian.

Exercise 19. Give an example of two Hermitian matrices whose multiplication is not Hermitian.

2.2 Unitary matrix

A matrix M is unitary if $MM^* = M^*M = I$. In other words, the columns of M form an orthonormal basis of the whole space. Unitary matrices need not be Hermitian, so their eigenvalues can be complex. For a unitary matrix, $M^{-1} = M^*$.

Exercise 20. Give an example of a unitary matrix which is not Hermitian.

Unitary matrices can be viewed as matrices which implement a change of basis. Hence they preserve the angle (inner product) between the vectors. So for a unitary M,

$$\langle u|v\rangle = \langle Mu|Mv\rangle.$$

Exercise 21. Prove the above equation.

That means unitary matrix preserves the norm of a vector and angle between vectors. Another way to characterize a unitary matrix is, they move any orthonormal basis to another orthonormal basis.

If two matrices A, B are related by $A = M^{-1}BM$, where M is unitary, then they are unitarily equivalent. If two matrices are unitarily equivalent then they are similar. Spectral theorem can be stated as the fact that normal matrices are unitarily equivalent to a diagonal matrix. The diagonal of a diagonal matrix contains its eigenvalues.

Exercise 22. What is the rank of a unitary matrix?

Note 7. Since unitary matrices preserve the norm, they will be used as operators in the postulates of quantum mechanics.

One of the important Unitary matrix is called the Hadamard matrix, it takes $|0\rangle$ to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|1\rangle$ to $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. You can compute the matrix representation and see that it satisfies $MM^* = I$.

Exercise 23. How can you show directly that it is a unitary matrix?

3 Evolution of a quantum system

The next postulate specifies, how a *closed* quantum system evolves. You might already know this postulate in terms of the very famous *Schrödinger's equation*. It is a partial differential equation which describes how a quantum state evolves with time.

The evolution is described by a *Hamiltonian* H which depends on the system being observed. For us, as computer scientists, it is just some Hermitian matrix H. Given the Hamiltonian H, the equation

$$i\frac{d|\psi\rangle}{dt} = H|\psi\rangle,$$

describes how the quantum system will change its state with time. For readers who are already familiar with this equation, we have assumed that Planck's constant can be absorbed in the Hamiltonian.

This equation can be considered as the second postulate of quantum mechanics. But, we will modify it a little bit to get rid of the partial differential equation and write it in terms of unitary operators.

Exercise 24. Read about Schrödinger's equation.

Suppose the quantum system is in state $|\psi(t_1)\rangle$ at time t_1. Then, using the Schrödinger's equation, the state at time t_2 is

$$|\psi(t_2)\rangle = e^{-iH(t_2-t_1)}|\psi(t_1)\rangle.$$

Exercise 25. Show that the matrix $e^{-iH(t_2-t_1)}$ is unitary.

Using the previous exercise,

$$|\psi(t_2)\rangle = U(t_2, t_1)|\psi(t_1)\rangle.$$

This gives us the "working" second postulate.

Postulate 2: A closed quantum system evolves unitarily. The unitary matrix only depends on time t_1 and t_2. If the state at t_1 is $|\psi(t_1)\rangle$ then the state at time t_2 is,

$$|\psi(t_2)\rangle = U(t_2, t_1)|\psi(t_1)\rangle.$$

Note 8. Unitary operators preserve norm and inner products.

Do you remember any unitary operators considered in this course before?

Exercise 26. Show that all Pauli matrices and the Hadamard matrix H are unitary operators.

Exercise 27. "Guess" the eigenvalues and eigenvectors of H. Check, if not, find the actual ones.

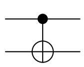
Notice that it is enough to specify the action of a gate/unitary on any basis, it is a linear operator. If we pick the standard basis, then we just need to mention the action on classical inputs. For example, Pauli X negates the classical inputs, it takes $|0\rangle$ to $|1\rangle$ and $|1\rangle$ to $|0\rangle$. That means, on any state $\alpha|0\rangle + \beta|1\rangle$, Pauli X will return $\alpha|1\rangle + \beta|0\rangle$. This is one of the preferred methods of specifying action of gates (or circuits) in quantum computing.

Another class of gates, useful in quantum computing, are the *controlled versions* of a unitary gate U. There are two inputs to these gates, one is the control part and other is the target part. The unitary U is applied to the target part if and only if the control part is in *ON* state. Mostly, if the control part is a set of qubits, setting all of them to be 1 is seen as the ON state.

The simplest and most useful of these gates is called the CNOT gate. It has one control and one target qubit.

Exercise 28. Suppose, first qubit is control and second qubit is target, write the matrix representation of CNOT gate.

The CNOT gate is drawn as,



Here the first qubit is control and second qubit is data.

4 Assignment

Exercise 29. Read about singular values of a matrix, show that the matrix M and M^* have the same singular values.

Exercise 30. Prove that the eigenvalues of a Hermitian matrix are real.

Exercise 31. Prove that the absolute value of the eigenvalues of an unitary matrix is 1. Is the converse true. What condition do we need to get the converse?

Exercise 32. Prove that a matrix M is Hermitian iff $\langle v|M|v\rangle$ is real for all $|v\rangle$.

Exercise 33. Show that the set of Hermitian matrices of a fixed dimension form a vector space (over which field?). What is the dimension of this vector space?

Exercise 34. Let $\sigma = \alpha_1 X + \alpha_2 Y + \alpha_3 Z$, where α_i's are real numbers and $|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 = 1$. Show that,

$$e^{i\theta\sigma} = \cos(\theta)I + i\sin(\theta)\sigma.$$

Exercise 35. Prove that if H is Hermitian then e^{iH} is a unitary matrix.

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