Lectures on Quantum Algorithms
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Mathematical Basics

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`https://en.wikipedia.org/wiki/Analytic_function_of_a_matrix\\`
`https://archive.siam.org/books/ot104/OT104HighamChapter1.pdf`

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Basic notions of quantum mechanics

Mathematical aspects

We will focus our attention here on operators acting on finite-dimensional spaces $\mathbb{H}$.

The set of vectors $\phi_j \in \mathbb{H}$ is **linearly independent** if for any finite subset

$$\phi_1, \phi_1, \ldots, \phi_n\}$$

and for $a_k \in \mathbb{C}$ the relation

$$a_2\phi_1 + a_2\phi_1 + \cdots + c_n\phi_n = 0$$

holds only if $a_1 = a_2 = \cdots = a_n = 0$. The space $\mathbb{H}$ is **finite dimensional** if $\mathbb{H}$ contains at most $n = \mathbb{H} < \infty$ linearly independent vectors. Otherwise $\mathbb{H}$ is infinite-dimensional.

The set of vectors $\phi_j \in \mathbb{H}$is said to **span** $\mathbb{H}$ if for any vector ϕ there exist $a_j \in$ such that:

$$\phi = \sum_j a_j \phi_j, \qquad \text{i.e.} \qquad \mathbb{H} = \text{Span}\{\phi_j | j = 1, \ldots, n\}.$$

Orthonormal basis $\{|e_j\rangle\}$ of $\mathbb{H}$ (bra-vectors):

$$|e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad |e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \cdots, \quad |e_n\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix},$$

Dual orthonormal basis $\{\langle e_j|\}$ of $\mathbb{H}$ (cket-vectors):

$$\langle e_1| = (1, 0, \ldots, 0), \quad \langle e_2| = (0, 1, \ldots, 0), \quad , \ldots, \quad \langle e_j| = (0, 0, \ldots, 1).$$

Vectors in $\mathbb{H}$:

$$\vec{z} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{pmatrix} = \sum_{j=1}^n z_j |e_j\rangle, \qquad \vec{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \sum_{j=1}^n w_j |e_j\rangle,$$

where $z_j, w_j \in \mathbb{C}$ are coordinates of the vectors $\vec{z}, \vec{w}$.

Scalar products of vectors:

$$\langle \vec{z} | \vec{w} \rangle = \langle \vec{z}^{\dagger} \vec{w} = \sum_{j=1}^{n} z_j^* w_j .$$

Obviously

$$\langle e_j | e_k \rangle = \delta_{jk} = \begin{cases} 1 & \text{if} \quad k = j, \\ 0 & \text{if} \quad k \neq j \end{cases} .$$

The coordinates of the vectors z_j and w_j are uniquely defined via:

$$z_j = \langle e_j | \vec{z} \rangle, \qquad w_j = \langle e_j | \vec{w} \rangle.$$

The length of the vectors:

$$||\vec{z}||^2 = \langle z | z \rangle = \sum_{j=1}^{n} |z_j|^2, \qquad ||\vec{w}|| = \langle w | w \rangle = \sum_{j=1}^{n} |w_j|^2.$$

$$\langle \vec{z} + \vec{w} | \vec{z} + \vec{w} \rangle = ||\vec{z}||^2 + ||\vec{w}||^2 + \langle \vec{z} | \vec{w} \rangle + \langle \vec{w} | \vec{z} \rangle.$$

Let us introduce two sets of indices $I = \{i_1, i_2, \ldots, i_k\}$ and $J = \{j_1, j_2, \ldots, j_m\}$ with $k + m \leq n$ and such that $I \cap J \equiv \oslash\emptyset$. Let us also introduce:

$$|\vec{z} = \sum_{j \in I} z_j |e_j\rangle, \qquad \vec{w} = \sum_{k \in K} w_k |e_k\rangle.$$

Then we have:

$$\langle \vec{z} | \vec{w} \rangle = 0, \qquad ||\vec{z}||^2 = \sum_{j \in I}^{n} |z_j|^2, \quad ||\vec{w}||^2 = \sum_{j \in K}^{n} |w_j|^2,$$

and therefore we obtain Pithagoras theorem:

$$\langle \vec{z} + \vec{w} | \vec{z} + \vec{w} \rangle = ||\vec{z}||^2 + ||\vec{w}||^2.$$

Linear maps on $\mathbb{H}$:

$$|\psi\rangle = \sum_{j} |e_j\rangle\langle e_j|\psi\rangle$$

Matrices can be written as:

$$A = \sum_{jk} |e_j\rangle\langle e_j|Ae_k\rangle\langle e_k| = \sum_{jk} |e_j\rangle A_{jk}\langle e_k|.$$

Thus the linear mappings on $\mathbb{H}$ are provided by matrices. They can also be viewed as linear operators on $\mathbb{H}$.

We introduce hermitian conjugation on the operator A:

$$(A^\dagger)_{jk} = ((A^T)^*)_{jk} = A^*_{kj}.$$

If

$$A^\dagger = A \qquad A \quad \text{is self-adjoint or hermitian} \qquad \text{Then} \qquad A_{jk} = A^*_{kj}$$

Then

$$(cA)^\dagger = c^* A^\dagger$$

The operator U is unitary, if:

$$\langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle \qquad \forall|\psi\rangle, |\phi\rangle \in \mathbb{H}.$$

This means that

$$UU^\dagger = U^\dagger U = \sum_j |e_j\rangle\langle e_j| = \mathbb{1},$$

where $\mathbb{1}$ is the identity operator on $\mathbb{H}$.

Eigenvectors of operators: The vector $|\psi\rangle$ is an eigenvector of A with eigenvalue $\lambda \in \mathbb{C}$ if:

$$A|\psi\rangle = \lambda|\psi\rangle.$$

All vectors $|\psi\rangle$ span an eigensubspace $\mathrm{Eig}(A, \lambda)$ of the operator A. The eigenvalue λ is non-degenerate if $\dim \mathrm{Eig}(A, \lambda) = 1$; If $\dim \mathrm{Eig}(A, \lambda) > 1$ the eigenvalue λ is degenerate.

The set of all eigenvalues λ_k of A is called the spectrum of A. If λ is an eigenvalue, then $(A - \lambda\mathbb{1})^{-1}$ does not exist.

$$\text{If} \qquad A|\psi\rangle = \lambda|\psi\rangle \qquad \text{then} \qquad \langle\psi|A^\dagger = \lambda^*\langle\psi|.$$

Prove that the eigenvalues of self-adjoint operators are real.
Prove that the eigenvalues of unitary operators have absolute value 1.

Self-adjoint operators are diagonalizable: Let

$$A|\psi_j\rangle = \lambda_j|\psi_j\rangle, \qquad \text{then} \qquad \langle\psi_j|A = \lambda_j\langle\psi_j|,$$

and

$$A = \sum_{j=1}^{n} \lambda_j |\psi_j\rangle\langle\psi_j|,$$

so if we choose as a basis the set of eigenvectors of A it becomes diagonal $\operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$.

Projectors. The operator P is called a projector if $P^2 = P$. If in addition $P = P^\dagger$ then P is an orthogonal projector.

Examples:

$$P_1 = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 \end{pmatrix}, \qquad P_2 = \begin{pmatrix} 0 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 \end{pmatrix}, \qquad P_1 + P_2 = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 \end{pmatrix}.$$

$$P_j = \frac{|\psi_j\rangle\langle\psi_j|}{\langle\psi_j|\psi_j\rangle}.$$

Properties of projectors:

$$P_j|\vec{z}\rangle = \frac{\langle\psi_j|\vec{z}\rangle}{\langle\psi_j|\psi_j\rangle}|\psi_j\rangle, \qquad \langle\vec{w}|P_j = \langle\psi_j|\frac{\langle\vec{w}|\psi_j\rangle}{\langle\psi_j|\psi_j\rangle},$$

Namely acting on any vector $|\vec{z}\rangle$ the projector produces vector proportional to $|\psi_j\rangle$.

$$A = \sum_{j=1}^{n} \lambda_j P_j.$$

For each orthogonal projector there is a set of orthonormal vectors $|\psi_j\rangle$ such that:

$$P = \sum_j |\psi_j\rangle\langle\psi_j| \qquad \text{iff} \qquad \langle\psi_j|\psi_j\rangle = 1.$$

From $P^\dagger = P = P^2$ deduce the eigenvalues of P.
A self-adjoint operator is called positive, if

$$\langle\psi|A|\psi\rangle \geq 0 \qquad \text{for all} \qquad |\psi\rangle \in \mathbb{H}.$$

We can introduce ordering of the operators and say, that $A > B$ if $A - B > 0$.

Another important operation between the operators is the commutator:

$$[A, B] = AB - BA.$$

If $[A, B] = 0$ we say that the operators commute.

Two commuting operators have the same set of eigenfunctions! This means, that they can be simultaneously diagonalized. However they may have different sets of eigenvalues, e.g.

$$A \Rightarrow \{\lambda_1, \lambda_2, \ldots, \lambda_n\}, \qquad B \Rightarrow \{\mu_1, \mu_2, \ldots, \mu_n\},$$

Check that any two diagonal matrices commute.

Properties of the hermitian conjugation:

$$(AB)^\dagger = B^\dagger A^\dagger.$$

Indeed,

$$(A.B)^\dagger = ((A.B)^T)^* = (B^T A^T)^* = (B^T)^*(A^T)^* = B^\dagger A^\dagger$$

Show that

$$\text{tr } A = \sum_k A_{kk} = \sum_k \langle e_k | A | e_k \rangle$$

does not depend on the choice of the orthonormal basis.
Show also that

$$\text{tr } (AB) = \text{tr } (BA).$$

Example: Let $\mathbb{H} \simeq \mathbb{C}^2$ – two-dimensional Hilbert space. We introduce an orthonormal basis by:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The dual orthonormal basis is:

$$\langle 0| = (1, 0), \qquad \langle 1| = (0, 1).$$

We introduce the operators $|x\rangle\langle y|$ where x and y take values 0 or 1. This gives:

$$|0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1, 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad |0\rangle\langle 1| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0, 1) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

$$|1\rangle\langle 0| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1, 0) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad |1\rangle\langle 1| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0, 1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

Prove that taking

$$|\phi\rangle = a|0\rangle + b|1\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \qquad |\phi\rangle = c|0\rangle + d|1\rangle = \begin{pmatrix} c \\ d \end{pmatrix},$$

we obtain a general operator in $\mathbb{C}^2$

$$|\psi\rangle\langle\phi| = (a|0\rangle + b|1\rangle)(c^*\langle 0| + d^*\langle 1|) = \begin{pmatrix} ac^* & ad^* \\ bc^* & bd^* \end{pmatrix}.$$

Pauli matrices and their tensor products

Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}_2.$$

Properties:

$$\sigma_k^2 = \sigma_0 = \mathbb{1}_2, \quad \sigma_k \sigma_j = i\epsilon_{kjm}\sigma_m, \qquad \{k, j, m\} = \{1, 2, 3\}$$

where ϵ_{jkm} is totally antisymmetric tensor, i.e.

$$\epsilon_{123} = 1, \qquad \epsilon_{kjm} = -\epsilon_{jkm} = \epsilon_{mkj}.$$

$$\sigma_1\sigma_2 = i\sigma_3, \quad \sigma_2\sigma_3 = i\sigma_1, \quad \sigma_2\sigma_1 = -i\sigma_3, \quad \sigma_3\sigma_2 = -i\sigma_1.$$

They appear when we need to describe the so-called spinor particles in quantum mechanics. An example of such particle is the electron which has spin 1/2. Pauli discovered that such particles may have only two states: the first one with spin up $|0\rangle$ and the second one with spin down $|1\rangle$. This nicely corresponds to the fact that in computers we use bites which also take two values.

Thus acting on bits we will have operators in $\mathbb{C}^2$ which are expressed in terms of Pauli matrices.

When we have two or more bites we will need tensor products of Pauli matrices:

$$\sigma_k \otimes \sigma_m, \qquad k, m = 0, 1, 2, 3;$$

These are 4×4 matrices of the form:

$$\sigma_0 \otimes \sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \qquad \sigma_1 \otimes \sigma_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},$$

$$\sigma_2 \otimes \sigma_k = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix}, \qquad \sigma_3 \otimes \sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix},$$

We can construct also triple tensor products of Pauli matrices

$$\sigma_k \otimes \sigma_m \otimes \sigma_j, \qquad k, m, j = 0, 1, 2, 3;$$

They have dimension 8.

Thus analyzing the action of the processors on the bites we will need operators whose matrix dimensions will be powers of 2.