Eigenvectors and Eigenvalues in Quantum Computing

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Eigenvalues and Eigenvectors

- Eigenvectors and Eigenvalues are special vectors/values that correspond to a matrix or linear transformation.
- They have important applications in various fields, including physics, computer science, and data analysis.

Intuition

Eigenvectors are vectors which change only by a scalar value (λ) after a linear transformation is applied to them. So if a linear transformation is applied to an entire subspace, there will be certain vectors in that subspace which do not move, but stay in place and only stretch by some scalar (λ).

Eigenvectors are the 'coordinate system' of a given matrix and the eigenvalues are the 'magnitudes' of each of the components of the coordinate system.

Definition

Let A be an $n \times n$ matrix. A scalar λ is an **eigenvalue** of A if there exists a non-zero vector $\mathbf{v}$ such that:

$$A\mathbf{v} = \lambda\mathbf{v}$$

Here, $\mathbf{v}$ is the **eigenvector** corresponding to λ.

Example: Eigenvalues

Consider the matrix

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$$

To find the eigenvalues, solve the characteristic equation:

$$\det(A - \lambda I) = 0 \tag{1}$$

$$\det\left(\begin{bmatrix} 3-\lambda & 1 \\ 1 & 3-\lambda \end{bmatrix}\right) = 0 \tag{2}$$

Expanding the determinant, we get:

$$(3-\lambda)^2 - 1 = 0$$

Solving for λ, we find two eigenvalues: $(3-\lambda)^2 - 1 = 0 \implies \lambda_1 = 2, \quad \lambda_2 = 4$

Example: Eigenvectors for $\lambda_1 = 2$

For $\lambda_1 = 2$, solve the system $(A - \lambda I)\mathbf{v} = \mathbf{0}$:

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Expanding, we get the system of equations:

$$\begin{cases} v_1 + v_2 = 0 \\ v_1 + v_2 = 0 \end{cases}$$

The solution is any vector in $\mathbb{R}^2$ with v_2 being arbitrary. Thus, the eigenvector is a scalar multiple of $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$.

Example: Eigenvectors for $\lambda_2 = 4$

For $\lambda_2 = 4$, solve the system $(A - \lambda I)\mathbf{v} = \mathbf{0}$:

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

The solution is a scalar multiple of $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$.

Applications

- **Diagonalization**: Diagonal matrices simplify matrix computations.
- **Principal Component Analysis (PCA)**: Used in data analysis and dimensionality reduction.
- **Quantum Mechanics**: Eigenvalues represent possible energy levels.
- **Google's PageRank Algorithm**: Eigenvectors help determine page rankings.

https://youtu.be/PFDu9oVAE-g?si=MweUnGVxJwko4t51

Eigenvalues and Eigenvectors [M2̈3]

- Computing the eigenvalues & eigenvectors of Hermitian and Unitary matrices is fundamental to QC & QM
- Computing eigenvalues & eigenvectors has an enormous number of applications in many different fields — especially science & engineering
- In the key quantum characterizations — matrices (Heisenberg) & waves (Schrödinger), eigenvalues & eigenvectors are foundational concepts

What is an observable in quantum mechanics?

- In QM, every variable is associated with an observable
- This is represented by a matrix
- The eigenvalues of this matrix tell us what possible values the variable can take when we measure it in an experiment
- One of the most important observables in physics is the Hamiltonian
- The Hamiltonian is associated with the energy which means the eigenvalues of the Hamiltonian tell us what possible values of energy we can measure in that system

Application: Simulating Molecules

- **Hamiltonian** — a matrix which describes the possible energies of a physical system. If we know the Hamiltonian, we can calculate the behaviour of the system
- **Eigenvectors** - A given physical system can be in various states.
- **Eigenvalues** - Each state has corresponding energies represented by eigenvalues.
- The lowest eigenvalue corresponds to the ground state energy.
- **Ground state** — this is the state of the system with the lowest energy, which means it's the "most natural" state — i.e. a given system always tend to get there, and if it is in the ground state and is left alone, it will stay there forever.

Lowest Eigenvalue

- In all physically relevant cases, the Hamiltonians have a lowest eigenvalue
- Physical systems have a lowest possible energy which is known as the ground state energy

$$E_0 \leq E_1 \leq E_2$$

- If the eigenvalues represent the possible values of the energy, what are the eigenvectors?
- The eigenvectors are states of the quantum system
- If a quantum system is in one of these "energy eigenstates", then measuring the energy of this eigenstate will yield the value of the energy (eigenvalue)
- If a quantum system is not in one of the energy eigenstates, then we get a some probablistic measurement outcomes

Application: Optimization Problems

- Finding lowest eigenvalues is crucial for tasks like portfolio optimization, logistics planning, and scheduling.
- A Hamiltonian can be used to describe an optimization problem
- The eigenvector corresponding to the lowest eigenvalue is an optimal solution to the problem

Eigenvalue Problems: Classical vs. Quantum

- **Classical Challenges**:
  - Computationally hard to find eigenvalues and eigenvectors classically.
  - Especially demanding for large, dense matrices due to algorithmic complexities.
- **Quantum Advantage**:
  - Quantum algorithms (e.g., QPE, VQE) offer potential advantages.
  - Expected to outperform classical methods for specific eigenvalue problems, providing a quadratic or exponential speedup.

Unitary Matrices/Transformation

- A quantum system evolves via unitary transformations
- Unitary matrices also have eigenvectors and eigenvalues

Given a unitary matrix (a quantum gate), U, and a corresponding eigenvector $|\psi\rangle$,

$$U|\psi\rangle = \lambda|\psi\rangle$$

Properties of Unitary Matrices

- **Eigenvalues** of a unitary matrix are complex and have a unit norm
- The eigenvalues lie on the unit circle in the complex plane
- Therefore, the exponential form of λ is given by $\lambda = e^{2\pi i\theta}$

$$U|\psi\rangle = e^{2\pi i\theta}|\psi\rangle$$

- **Eigenvectors** are orthogonal to each other

Eigenvalues and Eigenvectors of the Z-gate

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- has two eigenvalues $+1$ and -1
- corresponding to its eigenvectors $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Let's test it!

Why are the eigenvectors familiar?

Eigenvectors and eigenvalues of the X-gate

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- also has two eigenvalues $+1$ and -1
- corresponding to its eigenvectors $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ and $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$
- In Dirac Notation:
  - $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$
  - $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle$

Outer Products

$$|0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

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$$|0\rangle\langle 1| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$|1\rangle\langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$|1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Unitary matrices as outer products

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (1) * |0\rangle\langle 1| + (1) * |1\rangle\langle 0|$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = (-i) * |0\rangle\langle 1| + (i) * |1\rangle\langle 0|$$

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = (1) * |0\rangle\langle 0| + (-1) * |1\rangle\langle 1|$$

Outer product Dirac math

$$
\begin{aligned}
X|0\rangle &= (|0\rangle\langle 1| + |1\rangle\langle 0|)|0\rangle \\
&= |0\rangle\langle 1|0\rangle + |1\rangle\langle 0|0\rangle \\
&= |0\rangle(0) + |1\rangle(1) \\
&= |1\rangle
\end{aligned}
$$

$$
\begin{aligned}
X|1\rangle &= (|0\rangle\langle 1| + |1\rangle\langle 0|)|1\rangle \\
&= |0\rangle\langle 1|1\rangle + |1\rangle\langle 0|1\rangle \\
&= |0\rangle(1) + |1\rangle(0) \\
&= |0\rangle
\end{aligned}
$$

Spectral Decomposition

Since the eigenvectors form an orthonormal set, all unitary matrices can be written in a *diagonal representation* or an *orthonormal decomposition* (or equivalently, a *spectral decomposition*)

$$U = \sum_\lambda e^{2\pi i\theta_\lambda} |\psi_\lambda\rangle\langle\psi_\lambda|$$

where $e^{2\pi i\theta_\lambda}$ is the eigenvalue corresponding to the eigenvector $|\psi_\lambda\rangle$.

- This is also called the eigenbasis.

Example: Z-gate

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- has two eigenvalues $+1$ and -1
- corresponding to its eigenvectors $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

The spectral decomposition is:

$$Z = (1)|0\rangle\langle 0| + (-1)|1\rangle\langle 1| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + (-1)\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Applying Unitaries to its eigenvectors

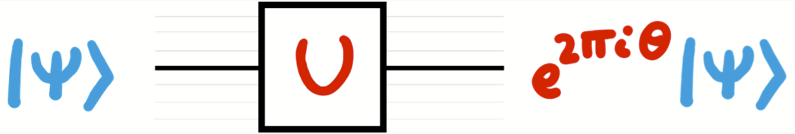
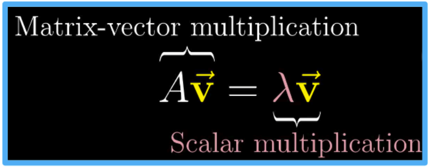
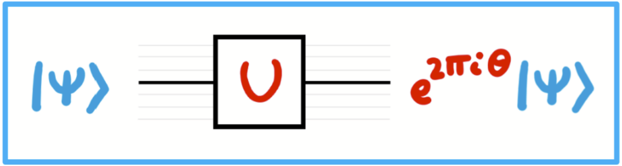


Figure 1: Applying a unitary to its eigenvector

Methods to find ground state energies: Quantum Phase Estimation (QPE) [M2̈3]





$$\underset{\text{Unitary Matrix}}{U}|\psi\rangle = e^{2\pi i\theta}|\psi\rangle$$

Estimate Phase θ

Compute Eigenvalue λ using θ

Eigen Value $\lambda = e^{2\pi i\theta}$

$$\ln\lambda = 2\pi i\theta$$

Phase Value $\theta = \dfrac{\ln\lambda}{2\pi i}$

References

Hausi Müller.
Course lectures on Quantum computing (UVic), 2023.