Gram-Schmidt Orthonormalization Process

Given a set of linearly independent vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}$, the Gram-Schmidt process constructs an orthonormal set $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_k\}$ using the following procedure:

$$\mathbf{e}_1 = \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|}$$

For each subsequent vector \mathbf{v}_i , subtract the projections onto the already constructed orthonormal vectors $\mathbf{e}_1, \ldots, \mathbf{e}_{i-1}$, and normalize:

$$\mathbf{e}_{i} = \frac{\mathbf{v}_{i} - \operatorname{proj}_{\mathbf{e}_{1}}(\mathbf{v}_{i}) - \cdots - \operatorname{proj}_{\mathbf{e}_{i-1}}(\mathbf{v}_{i})}{\|\mathbf{v}_{i} - \operatorname{proj}_{\mathbf{e}_{1}}(\mathbf{v}_{i}) - \cdots - \operatorname{proj}_{\mathbf{e}_{i-1}}(\mathbf{v}_{i})\|}$$

Where the projection of \mathbf{v}_i onto a vector \mathbf{e}_j is given by:

$$\operatorname{proj}_{\mathbf{e}_{j}}(\mathbf{v}_{i}) = \left(\frac{\langle \mathbf{v}_{i}, \mathbf{e}_{j} \rangle}{\langle \mathbf{e}_{j}, \mathbf{e}_{j} \rangle}\right) \mathbf{e}_{j}$$

Geometric Interpretation

The Gram-Schmidt process can be viewed as constructing orthogonal vectors step by step. The key idea is to iteratively remove the components of the vector that are parallel to the previously constructed orthonormal vectors.



Proof Outline

1. **Start with linearly independent vectors**: Assume $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}$ is a set of linearly independent vectors in an inner product space. 2. **First vector**: Set $\mathbf{e}_1 = \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|}$, which is clearly normalized.

3. **Inductive step**: Suppose we have constructed the orthonormal vectors $\mathbf{e}_1, \ldots, \mathbf{e}_{i-1}$. Define the projection of \mathbf{v}_i onto the span of $\{\mathbf{e}_1, \ldots, \mathbf{e}_{i-1}\}$ as:

$$\operatorname{proj}_{\operatorname{span}(\mathbf{e}_1,\ldots,\mathbf{e}_{i-1})}(\mathbf{v}_i) = \sum_{j=1}^{i-1} \langle \mathbf{v}_i, \mathbf{e}_j \rangle \mathbf{e}_j$$

4. **Construct \mathbf{e}_i **: Define the vector $\mathbf{v}'_i = \mathbf{v}_i - \operatorname{proj}_{\operatorname{span}(\mathbf{e}_1, \dots, \mathbf{e}_{i-1})}(\mathbf{v}_i)$. This vector \mathbf{v}'_i is orthogonal to all previous \mathbf{e}_j 's. Normalize \mathbf{v}'_i to get:

$$\mathbf{e}_i = rac{\mathbf{v}_i'}{\|\mathbf{v}_i'\|}$$

5. **Orthonormal set**: By construction, the vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_k$ are orthonormal.

Proof of the Cauchy-Schwarz Inequality

Let \mathbf{u},\mathbf{v} be vectors in an inner product space. We wish to prove the Cauchy-Schwarz inequality:

$$|\langle \mathbf{u}, \mathbf{v} \rangle| \le \|\mathbf{u}\| \|\mathbf{v}\|$$

Proof:

Consider the following expression:

$$\|\mathbf{u} - t\mathbf{v}\|^2 \ge 0$$
 for all real t

This inequality holds because the squared norm of any vector is always nonnegative. Now, expand the left-hand side:

$$\|\mathbf{u} - t\mathbf{v}\|^2 = \langle \mathbf{u} - t\mathbf{v}, \mathbf{u} - t\mathbf{v} \rangle$$

Using the properties of the inner product, this expands to:

$$= \langle \mathbf{u}, \mathbf{u} \rangle - 2t \langle \mathbf{u}, \mathbf{v} \rangle + t^2 \langle \mathbf{v}, \mathbf{v} \rangle$$
$$= \|\mathbf{u}\|^2 - 2t \langle \mathbf{u}, \mathbf{v} \rangle + t^2 \|\mathbf{v}\|^2$$

Since $\|\mathbf{u} - t\mathbf{v}\|^2 \ge 0$, this quadratic expression in t must be greater than or equal to zero for all values of t. Therefore, the discriminant of the quadratic equation must be non-positive. The discriminant of the quadratic is:

$$\Delta = (-2\langle \mathbf{u}, \mathbf{v} \rangle)^2 - 4 \cdot 1 \cdot \|\mathbf{v}\|^2 \|\mathbf{u}\|^2$$

Simplifying:

$$\Delta = 4\langle \mathbf{u}, \mathbf{v} \rangle^2 - 4 \|\mathbf{v}\|^2 \|\mathbf{u}\|^2$$

For the discriminant to be non-positive, we must have:

$$4\langle \mathbf{u}, \mathbf{v} \rangle^2 \le 4 \|\mathbf{u}\|^2 \|\mathbf{v}\|^2$$

Dividing both sides by 4:

$$\langle \mathbf{u}, \mathbf{v} \rangle^2 \le \|\mathbf{u}\|^2 \|\mathbf{v}\|^2$$

Taking the square root of both sides:

$$|\langle \mathbf{u}, \mathbf{v} \rangle| \le \|\mathbf{u}\| \|\mathbf{v}\|$$

Thus, we have proven the Cauchy-Schwarz inequality.

Grover's Algorithm: Overview and Connection to Gram-Schmidt and Cauchy-Schwarz Inequality

Grover's algorithm is a quantum algorithm designed to search an unsorted database or solve a black-box search problem with quadratic speedup compared to classical algorithms. It works by iteratively amplifying the amplitude of the target state, where the solution is encoded. In this explanation, we will show how the algorithm connects to two key mathematical tools:

- 1. Gram-Schmidt Orthonormalization to explain the iterative process of rotating quantum states.
- 2. Cauchy-Schwarz Inequality to quantify the change in amplitudes during each iteration and provide insight into the algorithm's performance.

Key Ideas in Grover's Algorithm

1. **Initial State**: Start with a quantum superposition of all possible states in the computational basis $\{|0\rangle, |1\rangle, \ldots, |N-1\rangle\}$, where $N = 2^n$ is the total number of possible states. The initial state is given by:

$$|\psi_0\rangle = \frac{1}{\sqrt{N}}\sum_{x=0}^{N-1}|x\rangle$$

2. **Oracle **: The oracle ${\cal O}$ marks the solution by flipping the phase of the target state:

$$O|x\rangle = (-1)^{f(x)}|x\rangle$$

where f(x) = 1 for the solution state x (the marked state), and f(x) = 0 for all other states.

3. **Amplitude Amplification**: Grover's algorithm repeatedly applies the **Grover operator**, which consists of two operations: - **Oracle Application**: Apply the oracle to flip the phase of the target state. - **Diffusion Operator^{**}: The inversion about the average operation amplifies the probability of the marked state.

The Grover operator G is given by:

$$G = (2|\psi_0\rangle\langle\psi_0| - I)O$$

The algorithm applies G repeatedly to amplify the amplitude of the target state. After approximately $\frac{\pi}{4}\sqrt{N}$ iterations, the state $|\psi\rangle$ is close to the marked state $|s\rangle$.

Mathematical Framework: Grover's Algorithm and Gram-Schmidt

We can view Grover's algorithm as iteratively projecting the initial quantum state onto a subspace that contains the target state, while maintaining the orthogonality of the quantum states in the process. The quantum state evolves in a two-dimensional subspace spanned by $|\psi_0\rangle$ and the solution state $|s\rangle$.

In this context, **Gram-Schmidt orthonormalization** helps explain the iterative process of rotating the quantum state towards the target state $|s\rangle$. At each iteration, the quantum state is adjusted to maintain the correct amplitudes while avoiding interference with non-target states.

We can define two subspaces: - S_{solution} : The subspace corresponding to the marked state $|s\rangle$. - $S_{\text{non-solution}}$: The subspace corresponding to all other states.

The Grover operator acts to rotate the initial state $|\psi_0\rangle$ towards $|s\rangle$, similar to applying an iterative Gram-Schmidt process. The operation increases the projection of $|\psi_0\rangle$ onto the subspace S_{solution} , while maintaining orthogonality with the non-solution subspace.

Mathematical Framework: Using the Cauchy-Schwarz Inequality

The Cauchy-Schwarz inequality provides a way to measure the change in the amplitude of the solution state after each Grover iteration. Suppose that after k iterations, the quantum state is $|\psi_k\rangle$. We can express the probability of measuring the solution state $|s\rangle$ as:

$$P_{\text{solution}} = |\langle s | \psi_k \rangle|^2$$

Let's define $\mathbf{u} = |\psi_k\rangle$ and $\mathbf{v} = |s\rangle$ as vectors in the Hilbert space. The Cauchy-Schwarz inequality tells us that:

 $|\langle s|\psi_k\rangle|^2 \le ||s\rangle||^2 ||\psi_k\rangle||^2 = 1$ (since both are normalized states)

The amplitude of the solution state after each iteration depends on the inner product between $|\psi_k\rangle$ and $|s\rangle$. Grover's algorithm iteratively increases this

inner product by applying the Grover operator, ensuring that the probability of measuring the target state grows over time.

At each step, the quantum state moves closer to $|s\rangle$ in the sense of the projection of the initial state onto the solution subspace. The inner product $\langle s|\psi_k\rangle$ quantifies this distance, and the amplitude amplification step ensures that this distance increases, eventually resulting in a high probability of measuring the solution.

Connecting Gram-Schmidt and Cauchy-Schwarz with Grover's Algorithm

- **Gram-Schmidt Parallel**: The process of rotating the quantum state towards the solution state can be viewed as an application of Gram-Schmidt orthonormalization. The quantum state is iteratively adjusted by subtracting out components in the subspace orthogonal to the solution state, thus increasing the component in the solution subspace. This orthogonalization process ensures that the algorithm avoids interference from non-solution states.

- **Cauchy-Schwarz**: The Cauchy-Schwarz inequality is essential to understanding the effectiveness of Grover's algorithm. It guarantees that the inner product $|\langle s|\psi_k\rangle|$ (the amplitude of the solution state) does not exceed 1 and provides a way to track how the amplitude grows with each iteration. By iteratively amplifying the amplitude of the target state, Grover's algorithm achieves a quadratic speedup over classical search algorithms.

Conclusion

Grover's algorithm leverages the concepts of **Gram-Schmidt orthonormalization** to iteratively rotate the quantum state towards the solution subspace and uses the **Cauchy-Schwarz inequality** to quantify the amplitude amplification process. The combination of these tools helps us understand the mathematical foundation of Grover's algorithm and why it provides a quadratic speedup for unstructured search problems.