Summary of Approach

In this work, I address the challenge of analyzing large-scale quantum circuits through the following steps:

Graph Representation of Quantum Circuits

The quantum circuit was represented as an undirected graph $G = (V, E)$, where the nodes V represent qubits and edges E represent two-qubit gates, specifically CZ or CNOT gates. The connectivity information was encoded using an adjacency matrix $A \in \mathbb{R}^{N \times N}$, where $A_{ij} = 1$ indicates an interaction (gate) between qubits i and j.

Graph Partitioning

The graph G was partitioned into multiple disjoint subgraphs $G_1, G_2, \ldots, G_k$ using community detection algorithms, with the goal of minimizing the number of edges between different subgraphs and maximizing intra-subgraph connectivity. This partitioning reduces cross-boundary entanglement, making the subsequent analysis of subcircuits more computationally feasible.

Quantum State Representation and Subcircuit Decomposition

The global quantum state $|\psi\rangle$ was represented as the tensor product of the quantum states of each subcircuit. For a quantum system divided into k subcircuits $A_1, A_2, \ldots, A_k$, the full quantum state can be expressed as:

$$|\psi\rangle = \sum_{\mathbf{i}} \alpha_{\mathbf{i}} \bigotimes_{j=1}^{k} |i_j\rangle_{A_j} ,$$

where $\mathbf{i} = (i_1, i_2, \ldots, i_k)$ are the indices corresponding to the states in each subcircuit, and $\alpha_{\mathbf{i}}$ are the complex amplitudes.

Schmidt Decomposition for Cross-Boundary Gates

For adjacent subcircuits that shared entangled qubits or had cross-boundary gates, we employed Schmidt decomposition to approximate the joint quantum state. Given a bipartite system composed of subcircuits A_i and A_j, the quantum state $|\psi_{A_i A_j}\rangle$ was decomposed as:

$$|\psi_{A_i A_j}\rangle = \sum_{k=0}^{r-1} \lambda_k |u_k\rangle_{A_i} \otimes |v_k\rangle_{A_j} ,$$

where λ_k are the Schmidt coefficients, $|u_k\rangle_{A_i}$ and $|v_k\rangle_{A_j}$ are orthonormal states of subcircuits A_i and A_j, respectively, and r is the Schmidt rank. To reduce the computational overhead, we truncated the decomposition by retaining only those Schmidt coefficients λ_k above a predefined threshold ϵ, effectively reducing the entanglement considered in the model.

Feature Extraction and Approximate State Reconstruction

Each subcircuit was simulated independently to extract key features. The extracted features included the probability distributions of the computational basis states, $p_i = |\alpha_i|^2$, and the entropy of the subcircuit state, calculated as:

$$S = -\sum_i p_i \log_2 p_i,$$

which quantifies the uncertainty or mixedness of the quantum state.

The approximate global quantum state $|\psi_{\text{approx}}\rangle$ was reconstructed by iteratively combining the state vectors of the subcircuits, while accounting for the truncated correlations across subcircuits:

$$|\psi_{\text{approx}}\rangle \approx \bigotimes_{j=1}^{k} |\phi_{A_j}\rangle ,$$

where $|\phi_{A_j}\rangle$ represents the state of subcircuit A_j after approximation.

Advantages of the Methodology

This methodology allows for the effective analysis of large-scale quantum circuits by:

- Reducing computational complexity through graph partitioning and parallel subcircuit analysis.
- Managing entanglement across subcircuits with Schmidt decomposition, making the problem more tractable.
- Employing statistical measures such as probability distributions and entropy, which provide meaningful insights without requiring full statevector storage.

Overall, this approach demonstrates the potential to handle circuits that are otherwise infeasible to simulate in their entirety, offering a scalable pathway for analyzing large quantum systems.