Toward Scalable Kernel-Based Quantum Machine Learning Using Tensor Networks

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Quantum Support Vector Machines (QSVMs) leverage quantum kernels to potentially outperform classical SVMs.[1] However, limitations in current quantum hardware—specifically in qubit count, circuit depth, and noise resilience—restrict their application to large-scale, real-world datasets. While simulating quantum circuits on high-performance computing platforms offers a promising alternative, classical simulation faces challenges due to exponential growth in matrix operation complexity ($\mathrm{O}(2^n)$ with qubit number) and quadratic scaling with data size ($\mathrm{O}(\mathrm{N}^2)$), in addition to severe memory constraints.

To address these issues, we propose a tensor network-based quantum kernel circuit simulation method that effectively overcomes the computational and memory bottlenecks associated with increasing qubit numbers and integrates parallelization techniques to enable QSVMs to operate on large-scale data.[2] Our approach begins by optimizing the data preprocessing pipeline to directly map input data into tensor network expressions, thereby reducing unnecessary overhead. We then perform a path search to determine the optimal matrix multiplication order, which minimizes computational complexity. Finally, we employ a shared computation pathway along with multi-GPU parallelization to accelerate operations.

Benchmark tests conducted on a national computing center's HPC platform demonstrate the efficacy of our method. On a single H100 GPU, our approach successfully simulates quantum circuits with over 60,000 qubits in approximately 73,148.36 seconds. Moreover, utilizing 32 H100 GPUs, we are able to simulate circuits with over 3,000 qubits for 1,000 data points in about 18,805 seconds.

In summary, this study highlights the potential of combining tensor networks with HPC to simulate large-scale QSVMs, overcoming current scalability limitations and paving the way for the application of quantum algorithms on extensive real-world datasets.

References

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