Toward Large-Scale-Qubit Quantum Circuit Simulation in Quantum Machine Learning with cuTN-QSVM

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The emergence of quantum computing has introduced significant potential for enhancing classical machine learning algorithms. One promising quantum-enhanced technique is the Quantum Support Vector Machine (QSVM), which leverages quantum kernel to explore substantial computational advantages over classical SVMs. In this paper, we present cuTensorNet-accelerated QSVM simulations, cuTN-QSVM for short, which leverage the computational capabilities of NVIDIA's cuQuantum SDK, specifically the cuTensorNet library, to achieve substantial speedup and enable larger-scale QSVM simulations on GPUs.

Our approach focuses on overcoming the primary computational bottlenecks associated with large-scale QSVM simulations, particularly the exponential growth in computational complexity with increasing qubit counts and quadratic growth in data sizes. Integrating the cuTensorNet library into the QSVM workflow for tensor-network-based simulations significantly reduces computational overhead, transforming previously infeasible simulations into manageable and parallelizable tasks, even across multiple GPUs in a distributed manner. Our experiments demonstrate that cuTensorNet enables the simulation of QSVMs with up to 10,000 qubits, a remarkable leap from the previous threshold of 50 qubits using state vector simulations.

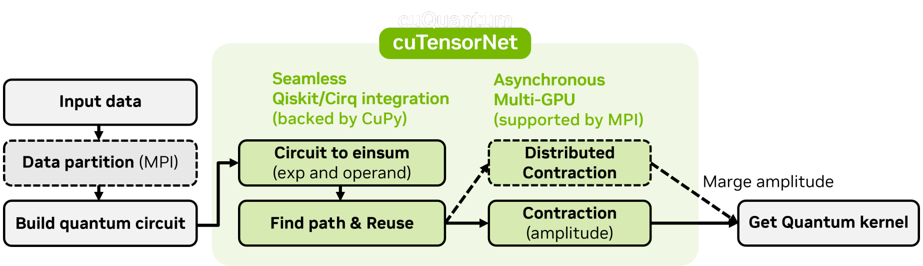

Figure 1: Optimizing QSVM simulation workflow with cuTensorNet in cuQuantum SDK streamlines the transition from circuit building to tensor network conversion and kernel matrix computation, reducing computational time via (multi-)GPU acceleration.

We employ a comprehensive simulation workflow that includes state preparation, quantum circuit transformation, and tensor network contraction. The cuTensorNet library's advanced features, such as path optimization and multi-GPU execution, allow us to perform these tasks efficiently on NVIDIA H100 GPU. Our evaluations show that the cuTensorNet-accelerated QSVM can complete simulations within seconds, even for qubit counts approaching 1000, and demonstrates strong linear speedup with increasing data sizes using multi-GPU processing and Message Passing Interface (MPI).

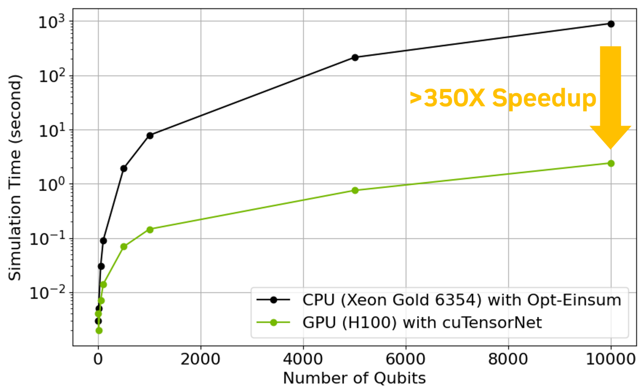

Figure 2: Benchmark QSVM circuit contraction time using a single CPU and a single GPU

Our study further explores the practical implications of these advancements, including a detailed analysis of computational complexity and resource requirements, even exceeding thousands of qubits. We provide benchmarking results that highlight the dramatic speedups achieved through GPU acceleration and the efficacy of the cuTensorNet library. Additionally, we discuss the implementation of a parameterized quantum circuit based on Block-Encoded State wavefunctions, which enhances the classification accuracy of QSVMs even with a greater number of qubits. In our talk, we will also introduce real-case studies, including image processing, and highlight the computational time analysis for practical applications of the cuTN-QSVM, showcasing its scalability on NVIDIA H100 GPUs.

The integration of cuTensorNet within the cuQuantum SDK accelerates QSVM simulations and opens new avenues for exploring complex quantum algorithms. Our work highlights quantum computing's potential to tackle large-scale machine learning challenges, marking a significant advance in quantum information science. Our future work includes implementing CUDA-Q, a unified programming platform for quantum computing research, to achieve more simplified usage and faster compile speed.

In conclusion, cuTN-QSVM represents a substantial advancement in quantum machine learning, leveraging state-of-the-art GPU acceleration to enable practical and efficient QSVM simulations. Our findings suggest that the cuTensorNet library will play a pivotal role in the future of quantum-enhanced machine learning, facilitating breakthroughs in both algorithm development and real-world data classification applications within the Quantum-HPC ecosystem.

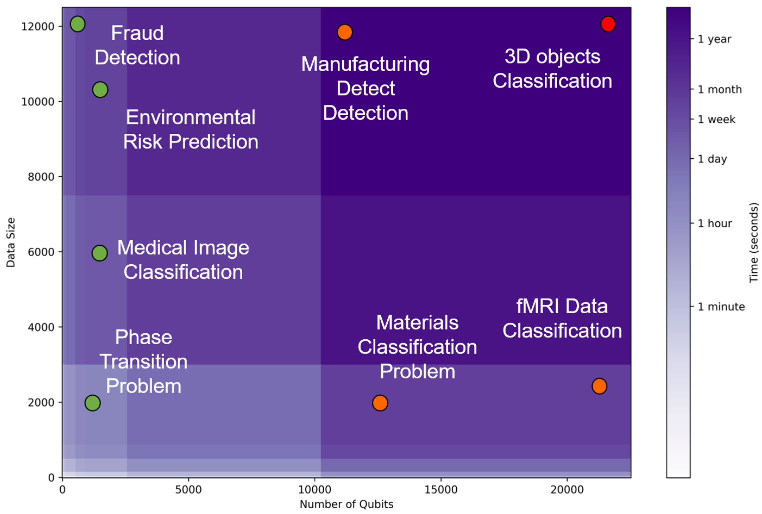

Figure 3: Resource estimation for solving different supervised learning problems using cuTN-QSVM with a 1 DGX cluster containing 8 x H100 NVIDIA GPUs

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