SAMPLE-BASED KRYLOV QUANTUM DIAGONALIZATION FOR OPTIMIZATION

IBM Quantum

Sample-based Krylov Quantum Diagonalization[1]

- Krylov diagonalization is a method by which the eigenpairs of a matrix may be approximated. Instead of diagonalizing the entire matrix, we do so in a smaller subspace generated by Krylov states; in the quantum case, these Krylov states can be $|\psi_k\rangle = e^{-ik\hat{H}\Delta t}|\psi_0\rangle$ for a Hamiltonian H and initial state $|\psi_0\rangle$.
- Sample-based quantum diagonalization is a quantum diagonalization method for systems with sparse ground states – meaning the ground state is a superposition dominated by relatively few basis states. By building an approximate ground state and sampling basis states to form a subspace, the ground state and energy can be approximated by projecting into said subspace and classically diagonalizing.
- These method can be combined into sample-based Krylov quantum diagonalization (SKQD), in which the subspace is built from samples taken from circuits generating Krylov states.

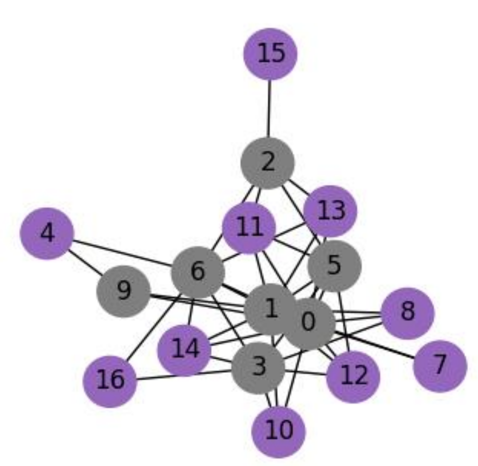
Pauli Correlation Encoding[2]

- Pauli correlation encoding (PCE) is a method of compression designed to work with variational quantum algorithms (VQAs) for performing quadratic unoptimized binary optimization (QUBO).
- PCE utilizes correlations between quantum states to decrease the required number of qubits in a quantum circuit to a maximum of $O(n^{1/2})$ for n variables
- Each bit value x_i is encoded as $sign(\langle\Pi_i\rangle)$ for a correlator Π_i, where is Π_i is the product of two identical Pauli matrices over two qubits (e.g., IXIXII for 6 qubits)

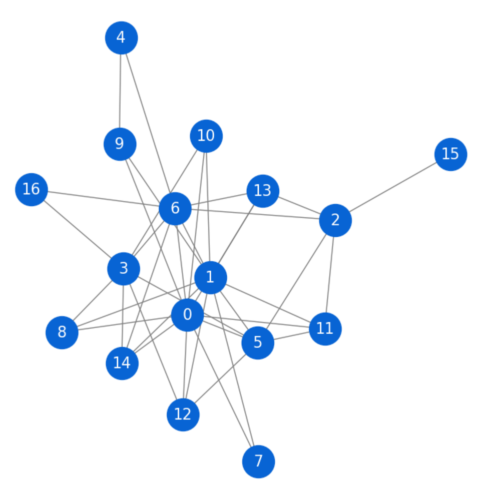
Maximum Independent Set

- Maximum independent set (MIS) is an NP-Hard constrained quadratic optimization problem with the goal of finding a graph's independent set – a set of nodes in which none are connected by an edge – with the maximum possible number of nodes.

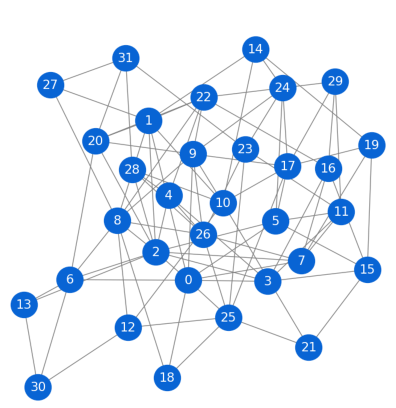
Graph[3]	Nodes	Edges	MIS Size
Farm	17	39	10
IBM32	32	94	13
Karate	34	78	20



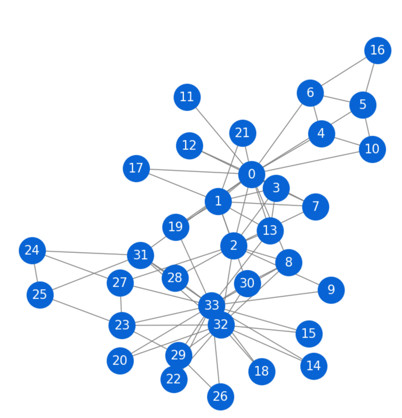
Farm graph MIS (purple)



Farm graph



IBM32 graph



Karate graph

PCE Setup for MIS

QAOA:

- Traditionally, the quantum approximate optimization algorithm (QAOA) is a VQA that uses an Ising Hamiltonian to generate approximate solutions to a given QUBO
- Here, we employ a flexible parameterized brickwork ansatz with a loss function to perform an approximate optimization as a benchmark for QAOA
- For positive constants M and L and with the first sum being over all edges and second over nodes, the problem can be captured with the following loss function:

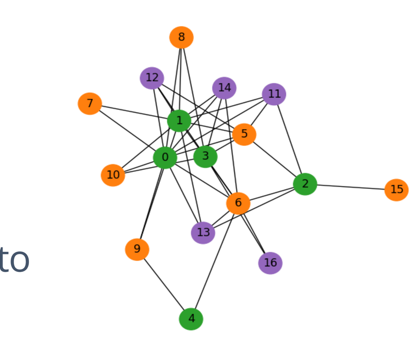
$$\mathcal{L} = M\sum_{(ij)} \frac{sgn(\langle\Pi_i\rangle)sgn(\langle\Pi_j\rangle)+sgn(\langle\Pi_i\rangle)+sgn(\langle\Pi_j\rangle)+1}{4} - L\sum_{i}\frac{sgn(\langle\Pi_i\rangle)+1}{2}$$

SKQD:

- Because SKQD generates Krylov states using the Hamiltonian, we require the PCE Hamiltonian to remain Hermitian.
- The approximate PCE Hamiltonian is

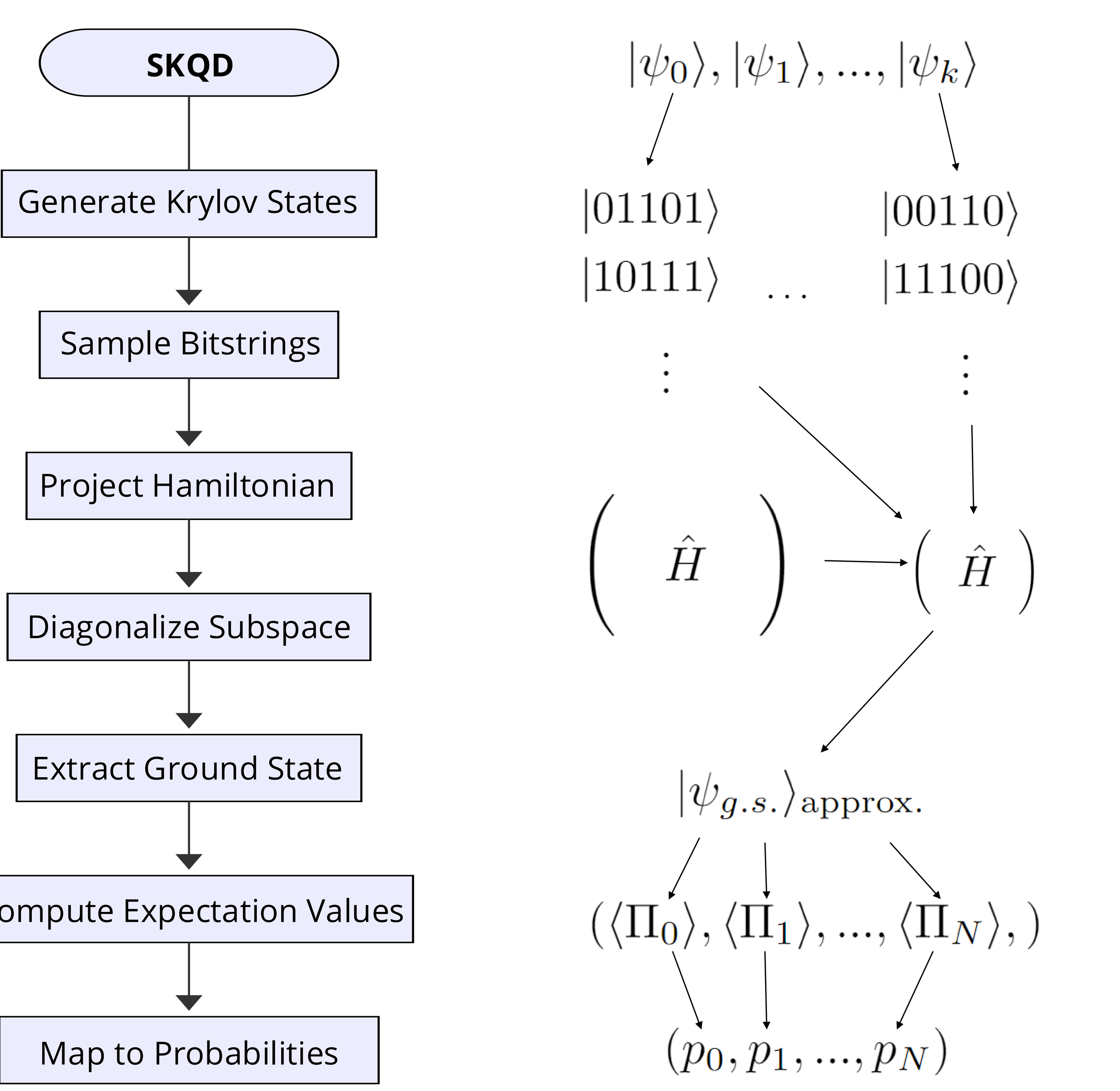
$$M\sum_{(ij)}\frac{\Pi_i\Pi_j+\Pi_i+\Pi_j+1}{4} - L\sum_{i}\frac{\Pi_i+1}{2}$$

- To avoid non-commuting correlators in the product term, we divide a graph into large independent sets to color our graphs. Within each set, we perform a separate encoding.
- Qubit compression decreases with increasing graph connectivity



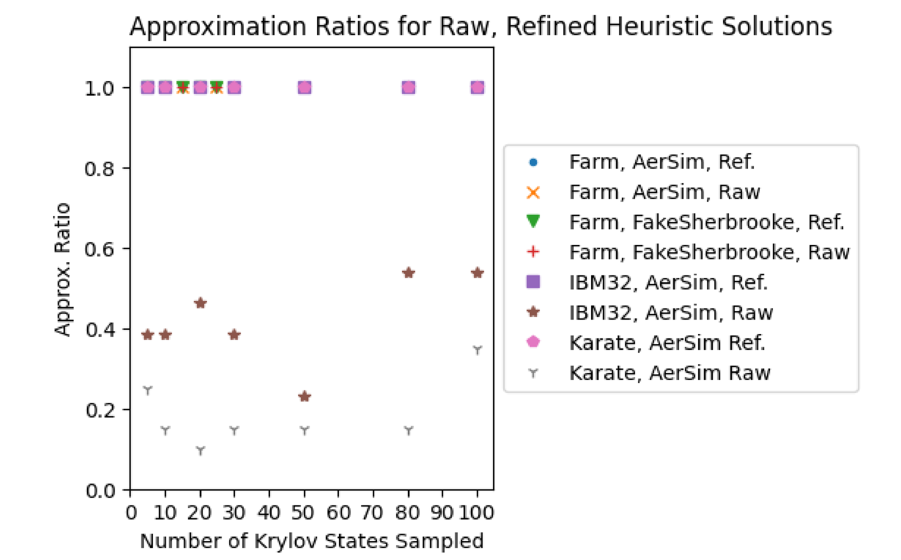
Farm graph coloring

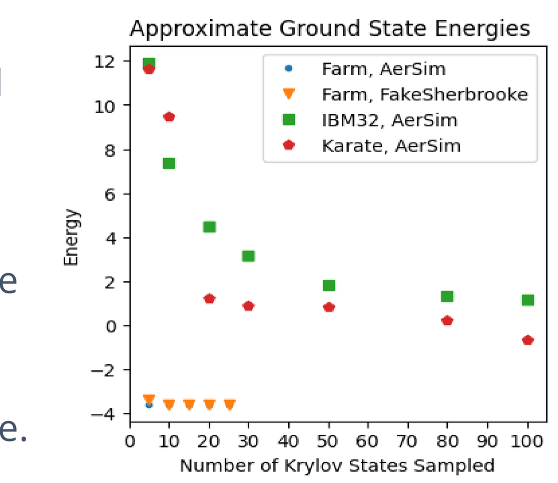
SKQD Workflow

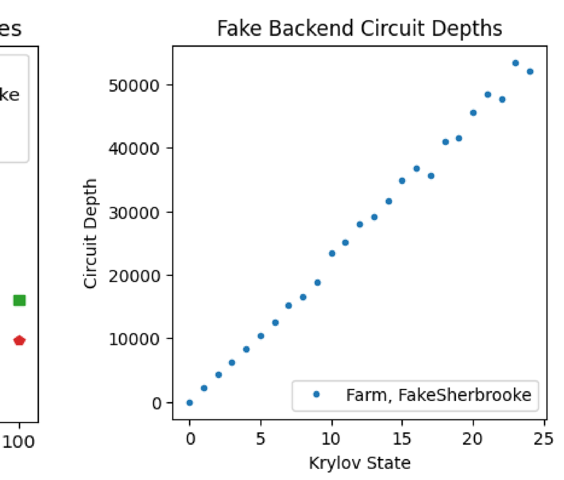


Results – SKQD, QAOA

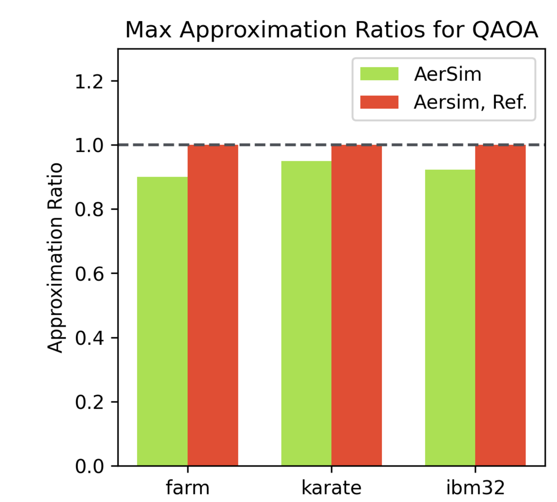
- Heuristic solutions were generated by adding bits to the set in order of decreasing probability until the set was no longer independent.
- Unrefined sets tend to have poor approximation ratios, but the refined sets all achieved an optimal MIS.
- For larger graphs, more Krylov states tend to be required for good ground state approximation.
- Circuit depths tend to increase linearly with k.
- Estimating 100 ns per gate operation, circuits with large k will likely require milliseconds of QPU usage.

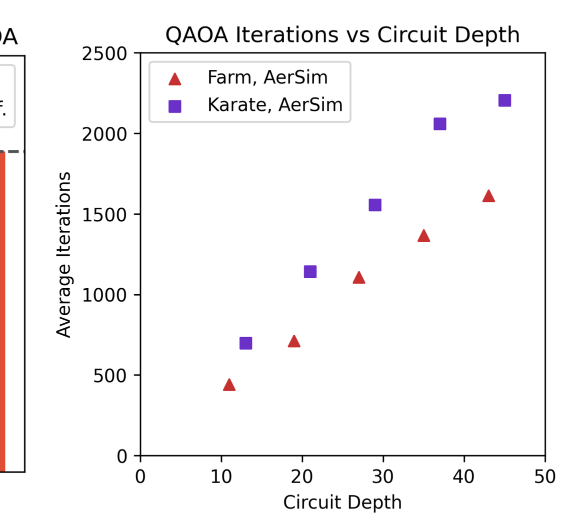


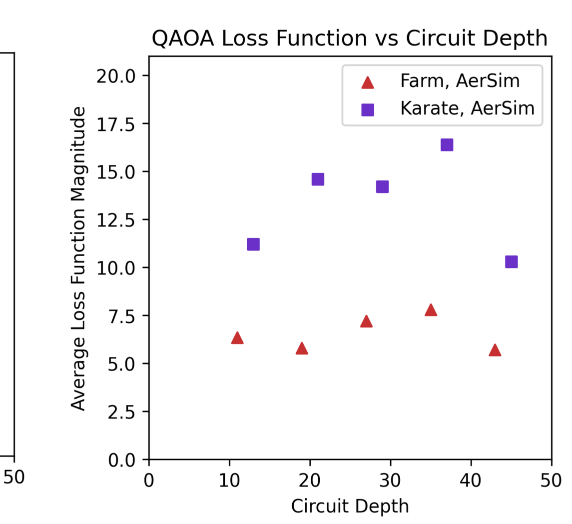




- For QAOA, the number of iterations increases with circuit depth
- Algorithm performance quantified by average loss function is sensitive to circuit depth
- Approximation ratios without refinement are >.9







Future Directions and References

- Sample-based methods with constraints can support configuration recovery – a method to recover invalid bitstrings based on information in valid bitstrings.
- Other classical optimization problems like max-cut are also good candidates for SKQD methods.
- Tuning Δt per graph could improve accuracy and reduce the number of Krylov states necessary for good solutions.

[1] Yu, J. et al. 2025. Sample-base Krylov Quantum Diagonalization. arXiv preprint arXiv:2501.09702v1 [quant-ph].
[2] Sciorilli, M. et al. 2024. Towards large-scale quantum optimization solvers with few qubits. arXiv preprint arXiv:2401.09421v2 [quant-ph].
[3] Koch, T. et al. (2025). Quantum Optimization Benchmark Library The Intractable Decathalon. arXiv preprint arXiv:2504.03832 [quant-ph].

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