# Some Results from HEP ML/Optimization Go Quantum

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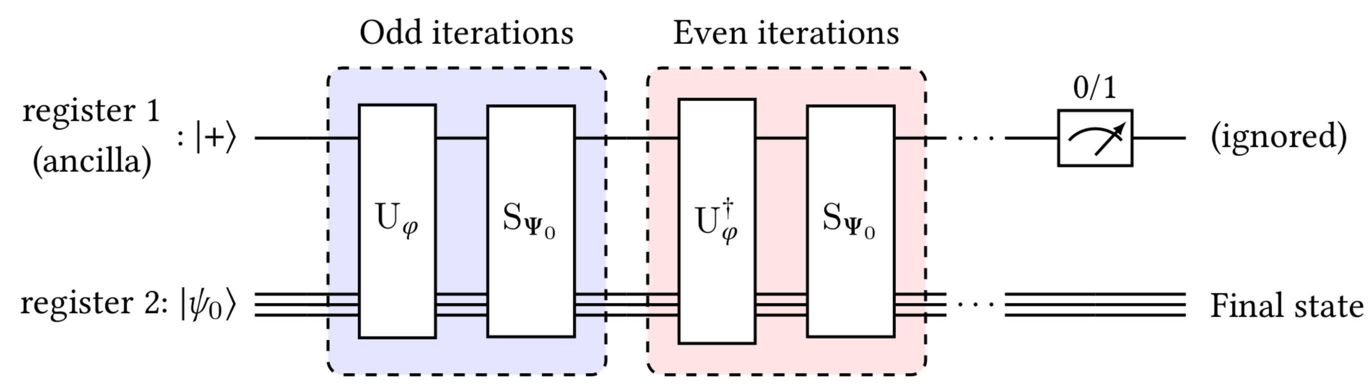
## Non-Boolean Quantum Amplitude Amplification and Mean Estimation

P. Shyamsundar, arXiv:2102.04975

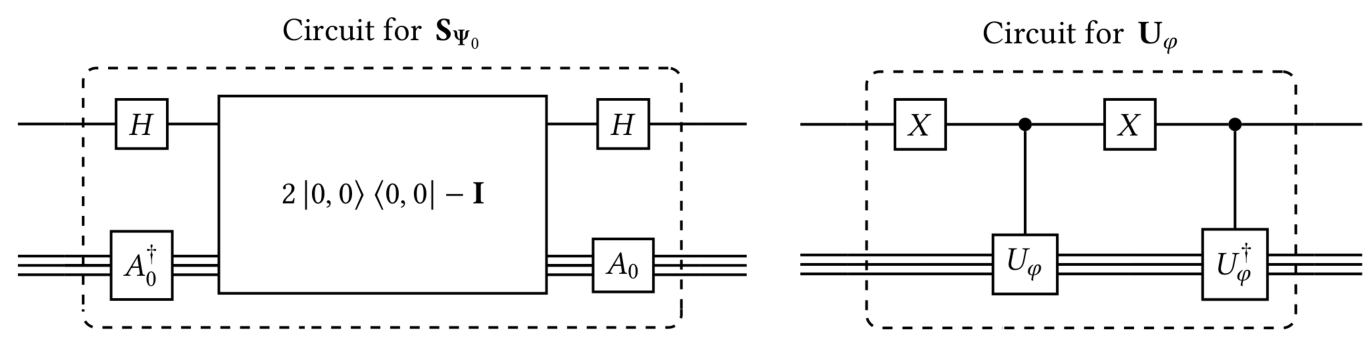
Grover's Algorithm amplifies the amplitude of "good" states, as judged by an oracle. $U_f|x\rangle = (-1)^{f(x)}|x\rangle$.

What if **goodness is on a non-Boolean scale**? $U_\varphi|x\rangle = e^{i\varphi(x)}|x\rangle$, where $\cos\varphi(x)$ signifies goodness (lower is better).

Grover's algorithm will fail. But non-Boolean amplitude amplification will work!

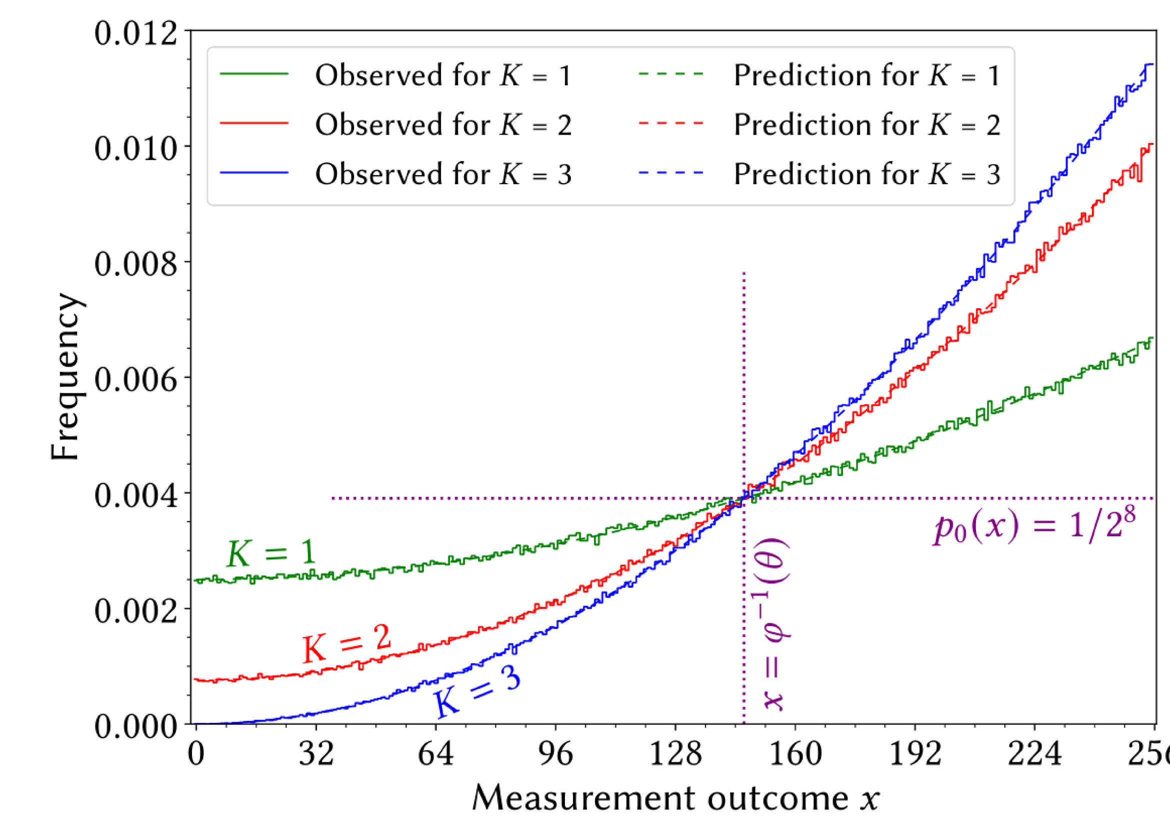



Quantum circuit for the non-Boolean Amplitude Amplification Algorithm




$$p_K(x) = p_0(x)\left\{1 - \lambda_K\left[\cos\big(\varphi(x)\big) - \cos(\theta)\right]\right\}$$

Expression for the amplified probabilities



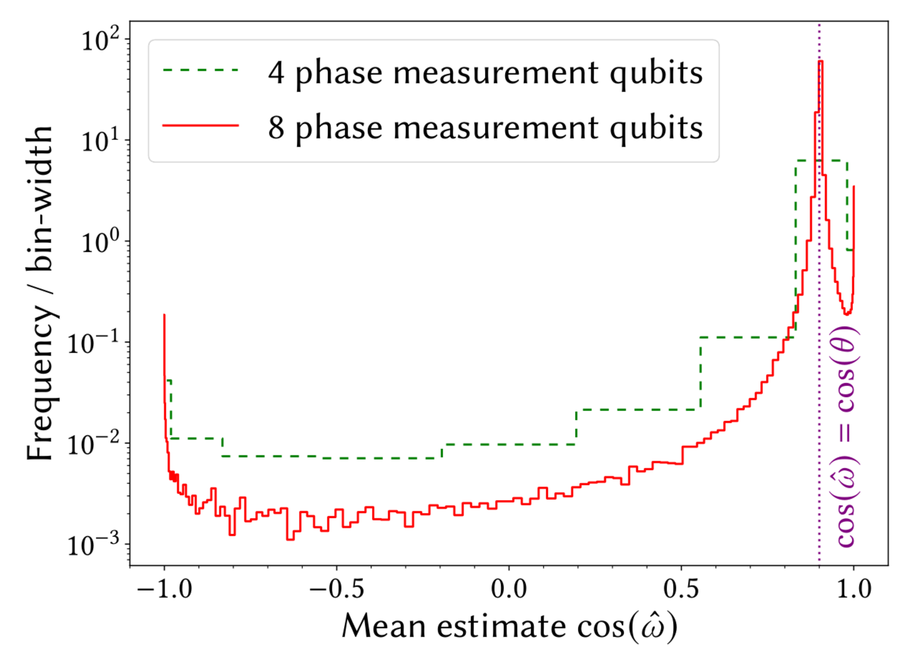

Measurement probabilities of states $|0\rangle, \ldots, |255\rangle$ after K=1, 2, and 3 iterations of non-Boolean amplification, for $\varphi(x) = \frac{x}{255}\frac{\pi}{4}$. Lower values of $\cos\varphi(x)$ have been preferentially amplified.

The quantum mean estimation algorithm can estimate $\langle\psi_0|U_\varphi|\psi_0\rangle$.

It uses quantum phase estimation. It is

- a by-product of the new non-Boolean amplification algorithm, and
- a generalization of the previously known amplitude estimation algorithm.

Offers quadratic speedup over shot-based estimation.




$\cos\theta$ is the real part of $\langle\psi_0|U_\varphi|\psi_0\rangle$. $\cos\hat{\omega}$ is the estimate for $\cos\theta$ from the mean estimation algorithm.

The histogram of $\cos\hat{\omega}$ peaks around $\cos\theta$. y-axis is on a log-scale.

### Outlook:

- Boolean amplitude amplification and estimation algorithms are widely applicable and feature as primitives in several quantum algorithms.
- The non-Boolean counterparts can be applied to a larger class of problems.
- Machine Learning applications of the algorithms are under investigation.

## Quantum Computing for Color Reconnections in High Energy Physics

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### Background:

Data analysis at HEP colliders proceeds via the comparison of real experimental data to data simulated under various theory models.

One of the stages of the simulation pipeline is the confinement of colored partons into colorless particles. Color reconnection is a heuristic idea used in the modeling of this confinement.

### Problem statement:

Given $n$ quarks and anti-quarks, and $m$ gluons find the valid arrangement of gluons that minimizes the $\lambda$ measure:

$$\lambda \equiv \sum_{i<j} \ln\frac{m_{ij}^2}{m_0^2} \equiv \sum_{i<j} w_{ij}$$

What is a valid assignment?

- All the particles are grouped into paths of the form $q \to g \to \cdots \to g \to \bar{q}$

### Converting to a QUBO problem:

One variable $x_{ij}$ for each edge in the problem.

$x_{ij}$ is 0 if an edge is inactive, 1 if active.

Energy function is given by:

$$E = \sum_{ij} w_{ij} x_{ij}$$

Constraints to avoid invalid assignments:

- Each quark and anti-quark is used exactly once

$$\sum_j x_{ij} = 1, \qquad \text{for } i \in \text{quarks and anti-quarks}$$

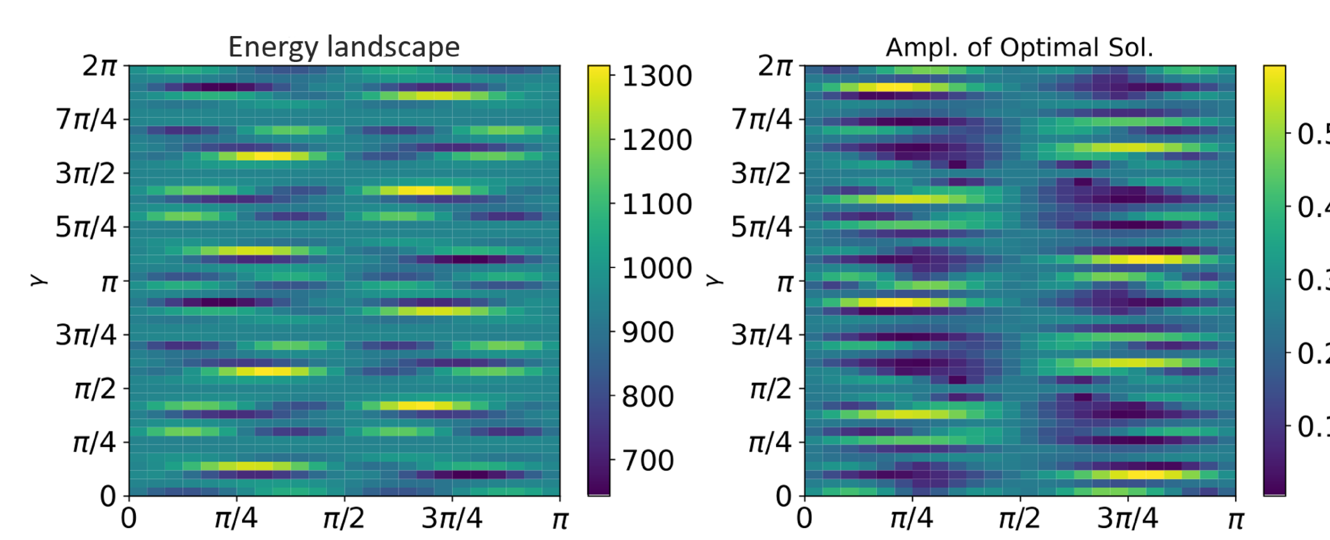
- Each gluon is used exactly twice

$$\sum_j x_{ij} = 2, \qquad \text{for } i \in \text{gluons}$$

Constraints are incorporated into QUBO using penalty terms

$$E = \sum_{ij} w_{ij}x_{ij} + \lambda \sum_{i \in Q \cup A}\left[1 - \sum_j x_{ij}\right]^2 + \lambda \sum_{i \in G}\left[2 - \sum_j x_{ij}\right]^2$$

This still doesn't avoid "subtours": "$q \to g \to \cdots \to g \to q$" or closed loops of gluons. Subtours can eliminated on a case-by-case basis.




Results from using QAOA to solve the color reconnection problem

### Outlook and Status:

- Exactly solving the color-reconnection problem leads to tangible effects in the simulated data for collider experiments. These can be experimentally validated, to improve our simulation models.
- The QUBO problems corresponding to color reconnection have almost full "connectivity" (large number of interaction terms). This makes QAOA hard to simulate beyond small toy problems.
- We are working on techniques to tackle large color reconnection problems a) using classical optimization techniques, b) on classical simulators of quantum computing, and c) near-term quantum hardware.

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