Investigation of Implementing Optimization-based Control of a CSTR using a Modified Grover's Algorithm with Inverse Sampling

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BACKGROUND:

» Model predictive control (MPC) and other advanced controllers are designed to…

- Solve an optimization problem utilizing a process model to minimize an objective function
- Find control inputs that maintain system within operating requirements

» This can be computationally expensive

- Quantum computing algorithms are appealing as can offer speedups in certain cases
- Not clear how control may benefit

» In [1]: utilized a modified Grover's algorithm to solve an optimization problem

- Objective function values calculated and encoded into oracle
- Gaussian solution space distribution is beneficial (see [2])
- Studied varying parameters in the algorithm, but this is not reliable for ensuring algorithm succeeds

» Investigate more systematic methods

- Investigate inverse sampling to transform uniform distribution to Gaussian

METHODS:

- Calculated distribution of objective function values for a continuous stirred-tank reactor (CSTR)
- Distribution transformed to a Gaussian using inverse sampling

RESULTS:

- Simulation of modified Grover's algorithm yielded high probability of success after inverse sampling

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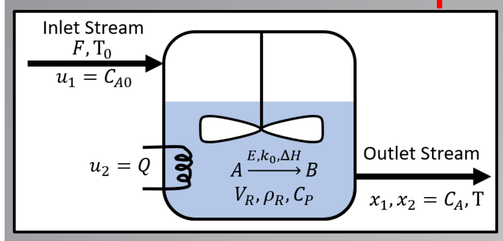
Solving control-based optimization problems using the modified Grover's algorithm still faces significant hurdles, but improved outcomes using inverse sampling motivates future research

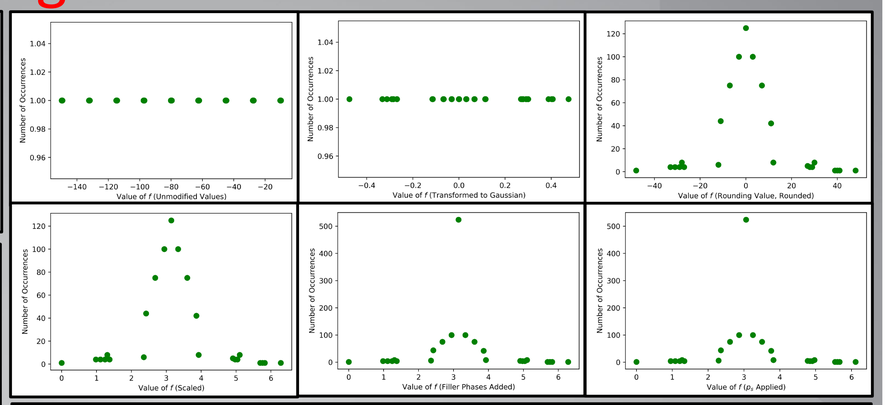


Continuous Stirred-Tank Reactor (CSTR):

- Single inlet, single outlet
- Exothermic reaction of A to B

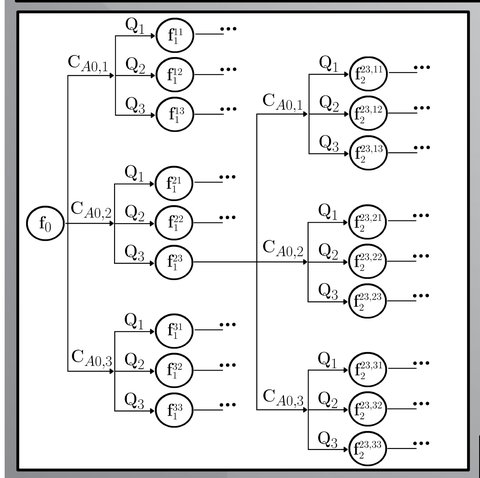
$$\frac{dC_A}{dt} = \frac{F}{V_R}(C_{A0} - C_A) - k_0 e^{-E/RT} C_A^2$$

$$\frac{dT}{dt} = \frac{F}{V_R}(T_0 - T) - \frac{\Delta H k_0}{\rho_R C_p} e^{-E/RT} C_A^2 + \frac{Q}{\rho_R C_p V_R}$$



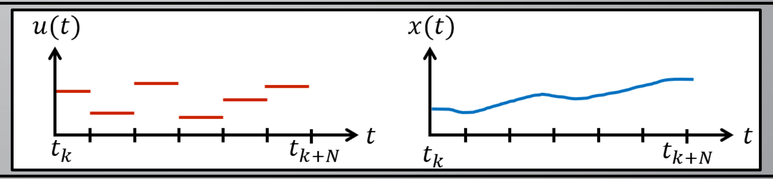
Creating a Distribution:

1. Calculate objective function values using branching tree scheme
2. Inverse Sampling
3. Round
4. Scale from 0 to 2π
5. Add filler phases to ensure 2^n phases exist
6. Apply p_s



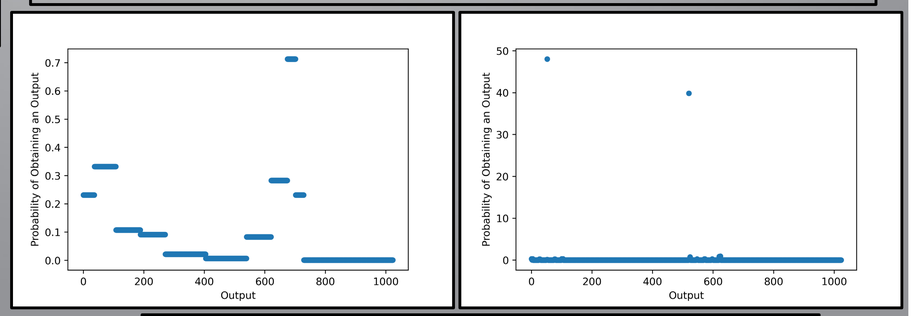
Solution Space:

- Important to consider because algorithm success depends highly on the solution space distribution
- Created using a branching tree scheme
- Objective functions values calculated by classical means and used in the oracle in a quantum computing simulation



Model Predictive Control (MPC):

- Assumes inputs are applied sample-and-hold over each sampling period
- Predicts optimal inputs to maximize objective over N sampling periods
- Objective function: $f = \int_{t_k}^{t_{k+N}} \left[-k_0 e^{-E/RT(t)} C_A(t)^2 - 0.1 C_{A0}(t) - 10^{-12} Q(t)^2\right]$



Example of results before inverse sampling (left) and results after inverse sampling (right). Probabilities are in percent.

Approved for Public Release; Distribution Unlimited: AFRL-2023-3645

INVERSE SAMPLING:

Method of transforming samples taken from one distribution to be as if they were taken from a different distribution

- In this work, treat the objective function values as a uniform distribution, scaling the values to be in the range $(0,1)$
- Transform to a Gaussian distribution to increase effectiveness of amplitude amplification

$$y = \mu - \sigma\sqrt{2}\,\mathrm{erf}^{-1}(2x - 1)$$

$x =$ A point taken from a uniform distribution

$y =$ Corresponding point from a Gaussian distribution (with mean μ and standard deviation σ)

CONCLUSIONS:

- Demonstrates there may be methods of solution space manipulation to improve the outcome of the modified Grover's algorithm
- In the future, it is important to determine an efficient and *a priori* method
- For the algorithm to demonstrate quantum supremacy, preprocessing of data must not negate the advantage gained using amplitude amplification

REFERENCES:

[1]. Nieman, K., Durand, H., Patel, S., Koch, D., Alsing, P. "Investigating an Amplitude Amplication-Based Optimization Algorithm for Model Predictive Control." Digital Chemical Engineering. Submitted 2023.

[2]. Koch, D., Cutugno, M., Karlson, S., Patel, S., Wessing, L., and Alsing, P. "Gaussian Amplitude Amplification for Quantum Pathfinding." arXiv preprint arXiv:2112.08167, 2021.

[3]. Benchasattabuse N., Satoh T., Hajdušek M., and Van Meter, R. "Amplitude Amplification for Optimization via Subdivided Phase Oracle." 2022 IEEE International Conference on Quantum Computing and Engineering (QCE). IEEE, 2022.

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