University of Stuttgart
Institute for Computational Physics

SimTech

Topical Meeting – Machine Learning

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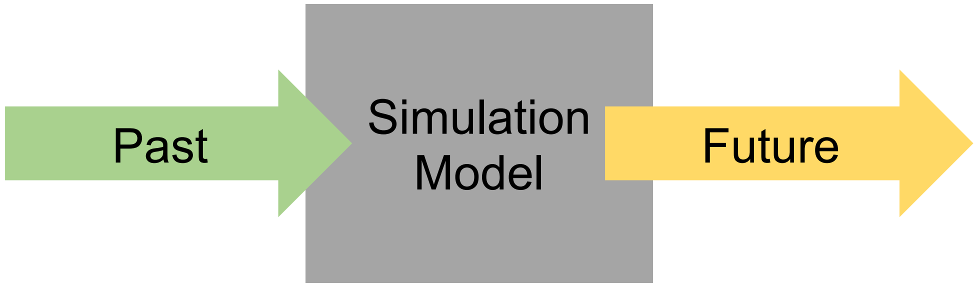
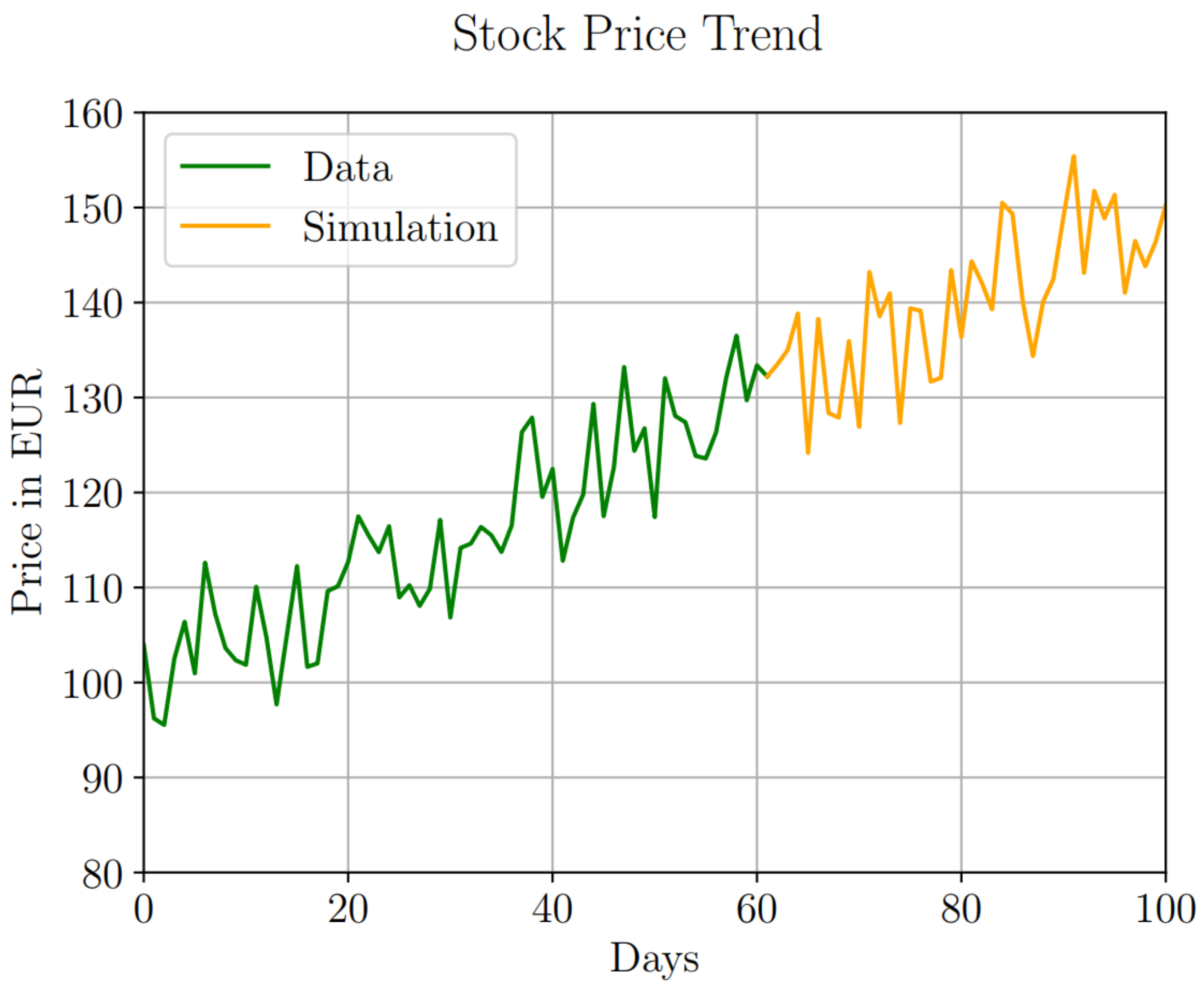
Simulating Stochastic Processes with Quantum Devices

May 17th, 2023

Stochastic Processes

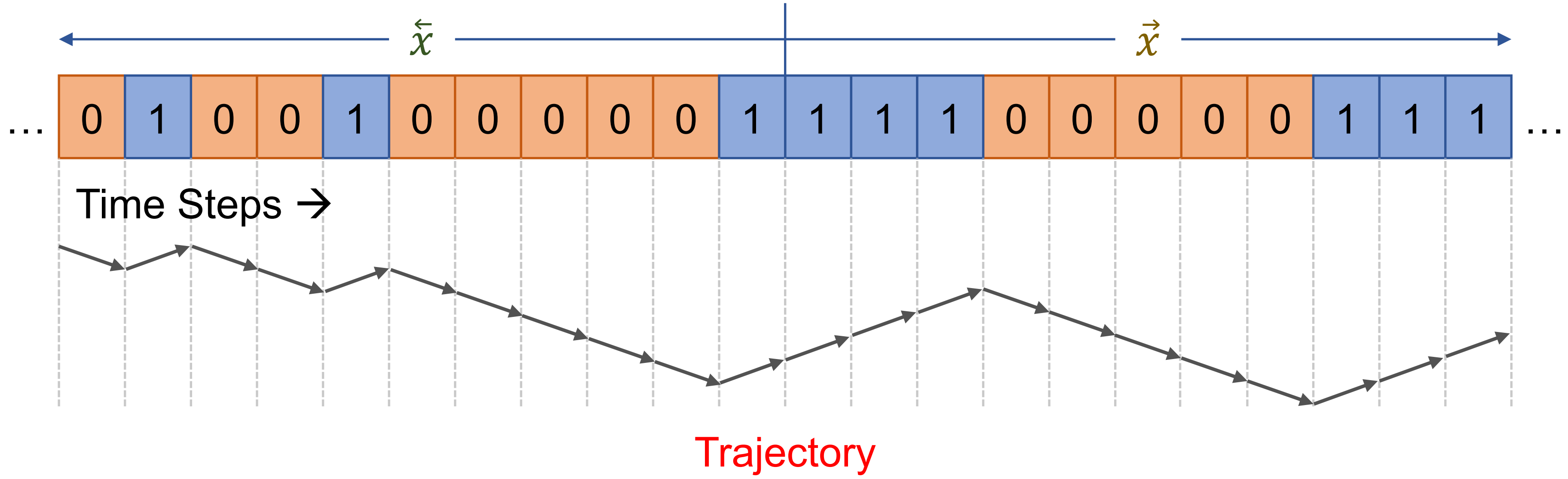
Assume data drawn
by a stochastic process





Stochastic Processes

- Simulating = sampling trajectories
- Trajectory is governed by $P(\vec{X}|\overleftarrow{X})$



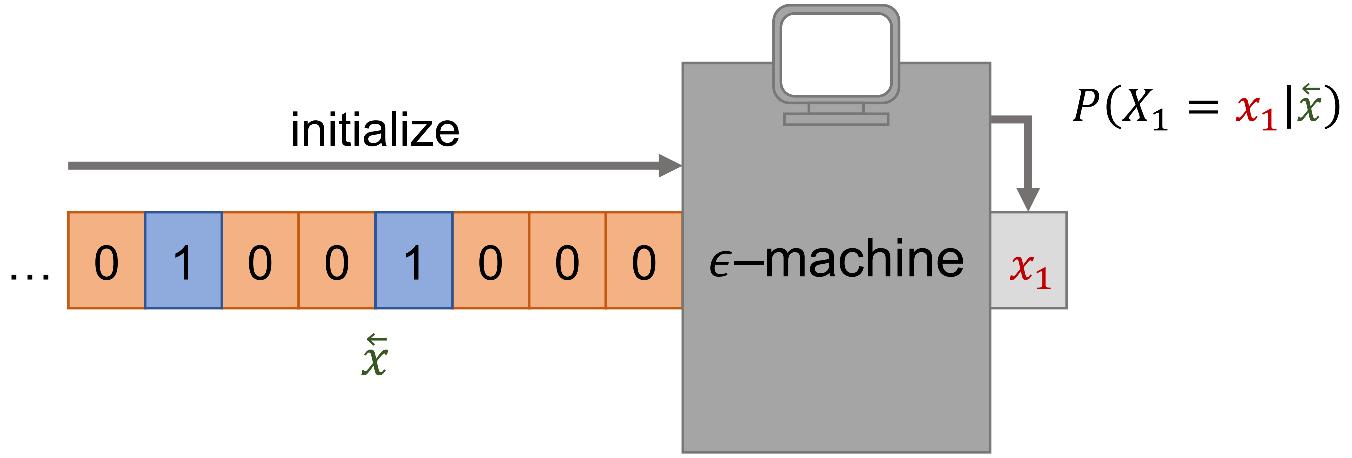
Simulation Models

Quantum models use **less memory**

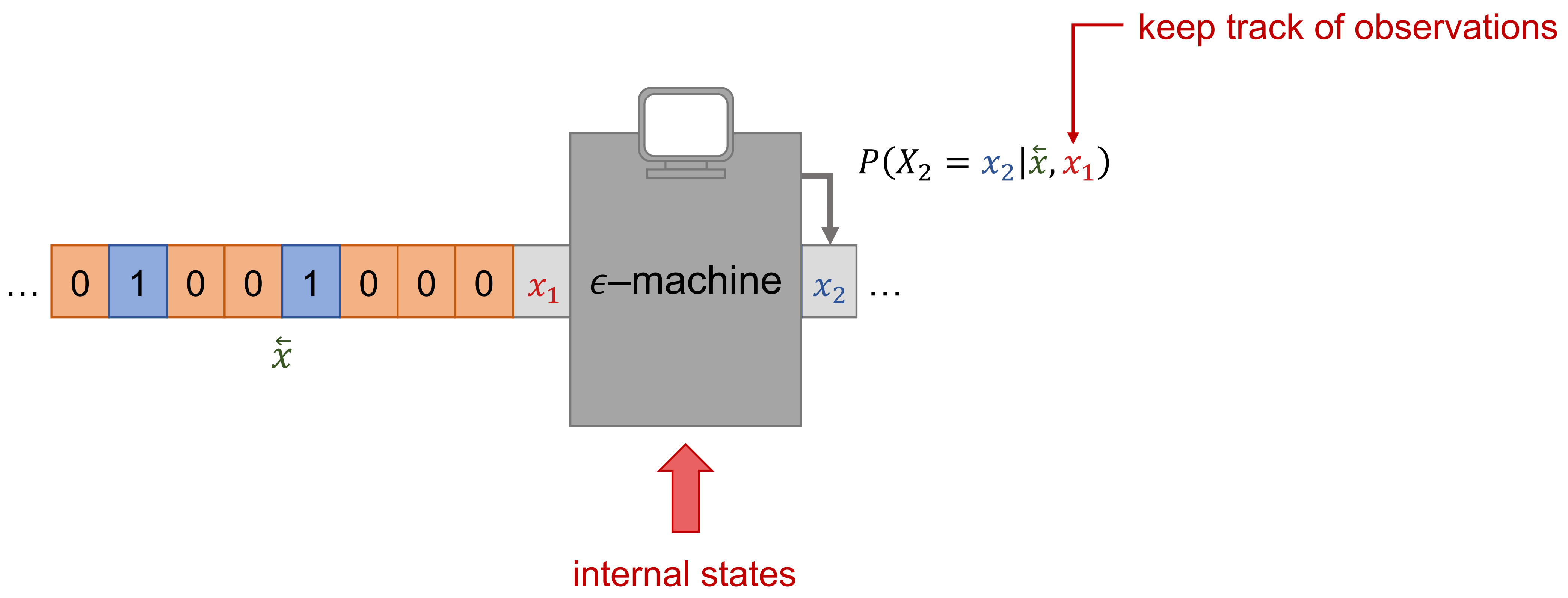
→ simulate complex processes more easily

→ approximate complex processes more accurately

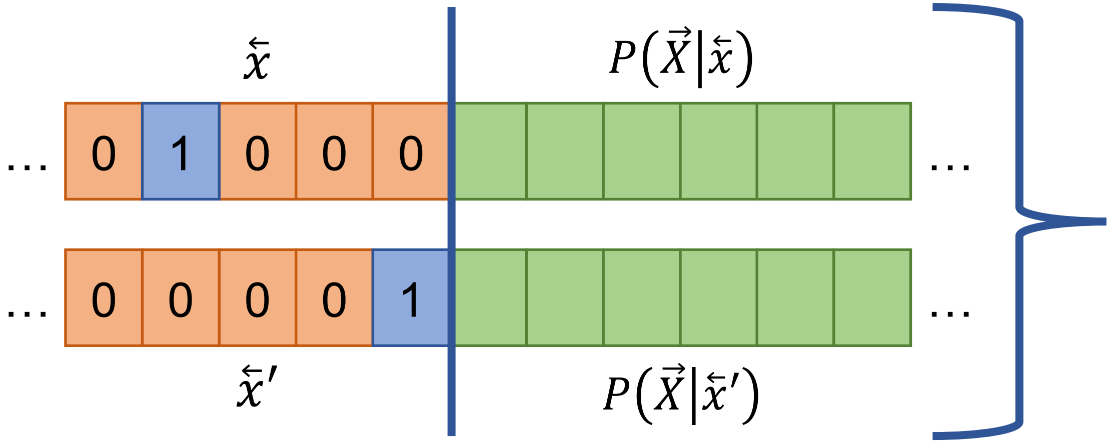
ϵ–Machine



ϵ–Machine



ϵ–Machine



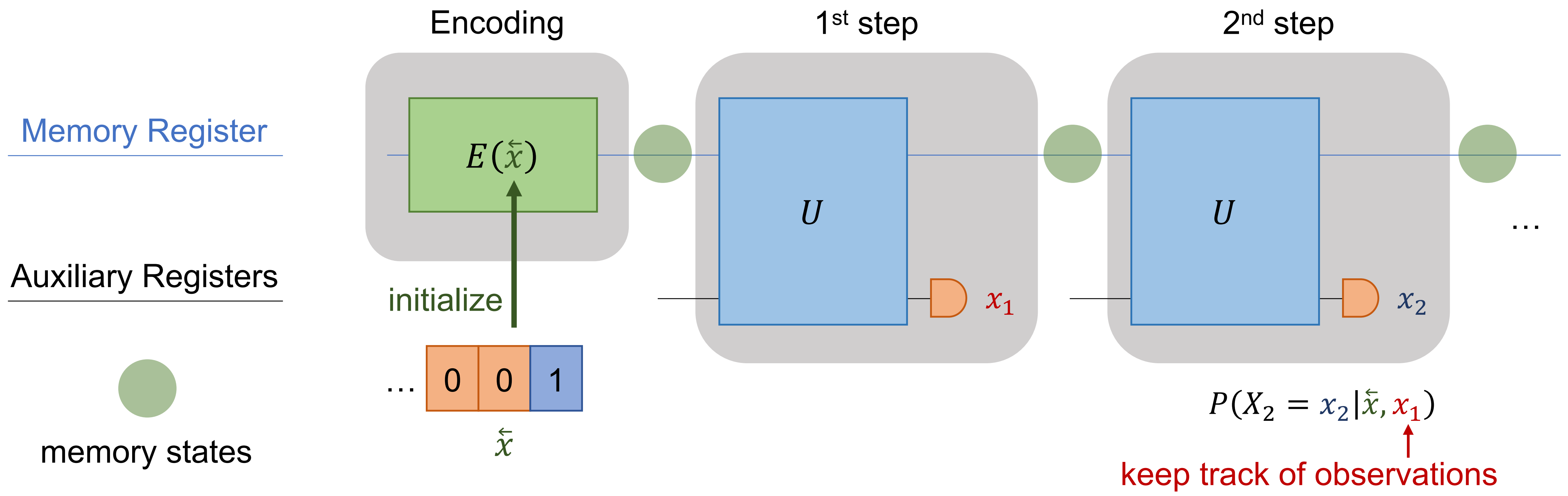
$\overleftarrow{x} \sim \overleftarrow{x}' \Leftrightarrow P(\vec{X}|\overleftarrow{x}) = P(\vec{X}|\overleftarrow{x}')$

causal sates $\{s_i\}_{i=1}^{N}$ (minimal)

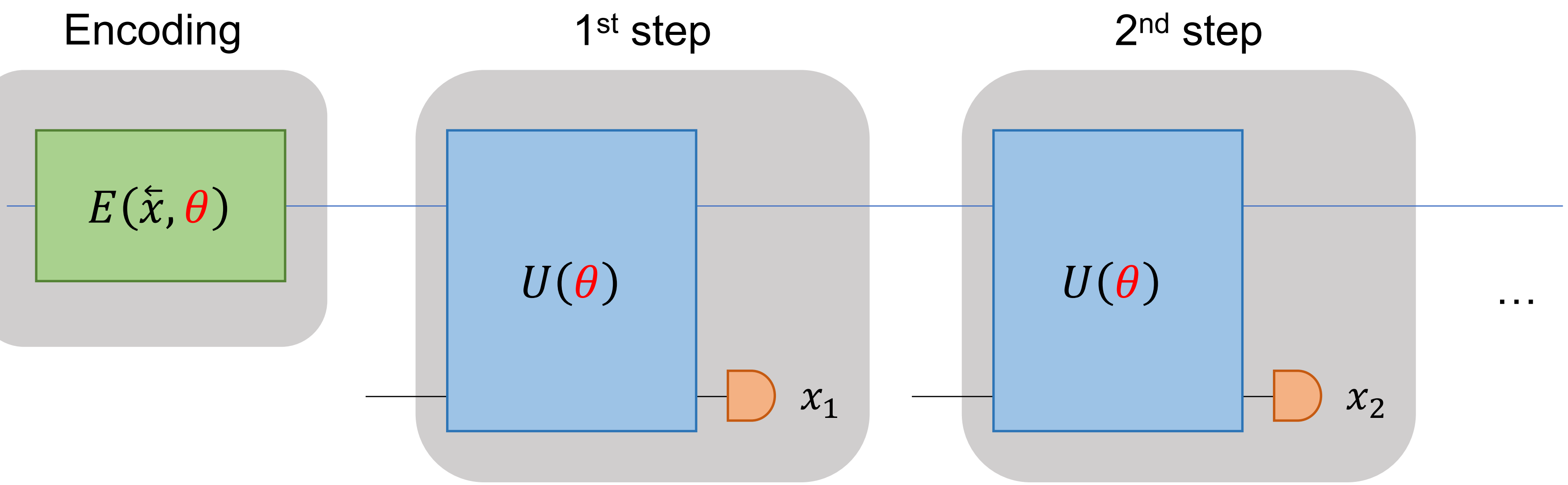
map $E(\overleftarrow{x}) = s_i$ (Initialization)

Classical Topological Complexity: $d_c = \log_2 N$

q–Simulator



Quantum Topological Complexity: $d_q = \#\text{qubits}$



$P_\theta(X_2 = x_2 | \overleftarrow{x}, x_1)$

Approximate P → $|P - \hat{P}_{\boldsymbol{\theta}}| < \delta$

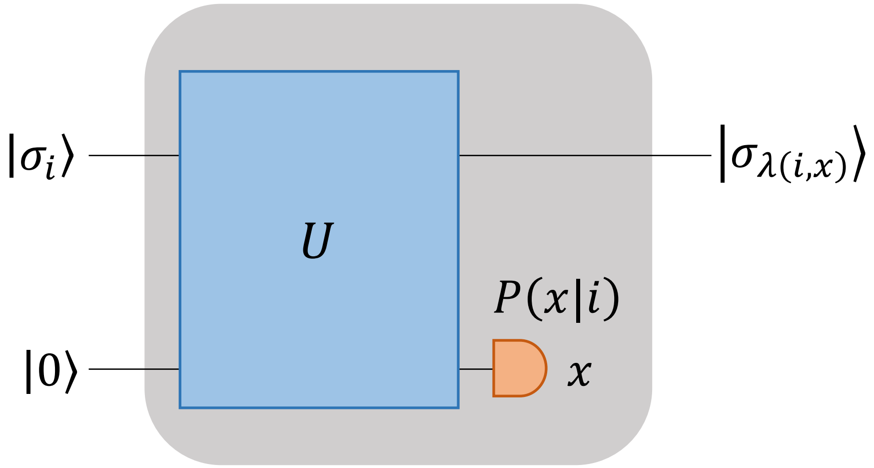
Obstacles

- “Brute-force learning” doesn’t work for slightly more complex processes
- Tailor-made ansätze are required, but hard to engineer
- A fundamental theory behind the “approximation” is missing

→ Create a (mathematical) framework for approximate quantum models

→ “Low-rank approximations of unitary simulators”

Notation

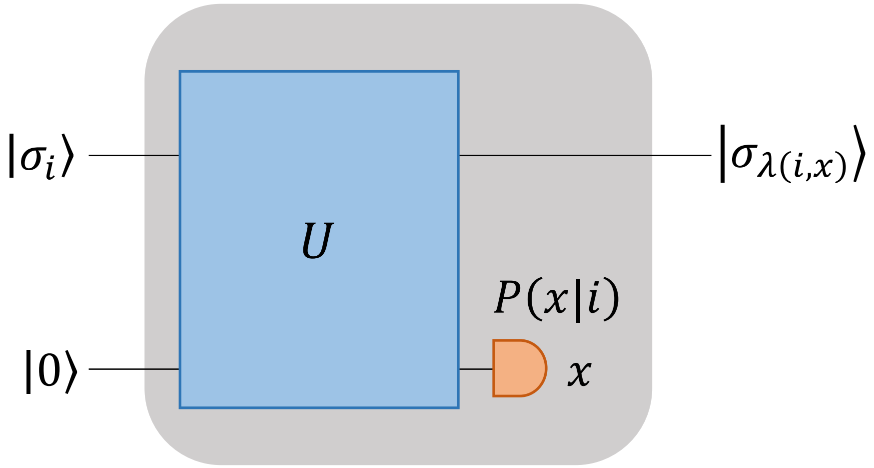


- dynamics $\lambda(s_i, x) \in \{0,1,\dots,N\}$

- Joined state after one simulation step:

$$|1_i\rangle = U|\sigma_i\rangle|0\rangle = \Sigma_x \sqrt{P(x|i)}\,|\sigma_{\lambda(i,x)}\rangle|x\rangle$$

Notation



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assume to be given

Theorem

There exists a q-Simulator U with memory states $|\sigma_i\rangle$ iff

$$\langle\sigma_i|\sigma_j\rangle = \langle 1_i|1_j\rangle \quad \text{for all} \quad i, j.$$

Note this is independent of the number of memory/auxiliary qubits.

Additionally, note that $\langle 1_i|1_j\rangle = \sum_{x_\infty} \sqrt{P(x_\infty|i)P(x_\infty|j)}$

Binder et al., 10.1103/PhysRevLett.120.240502

→ Main idea: perform a *low-rank approximation* of $C_{ij} = \langle 1_i|1_j\rangle$

Algorithm

1. Construct the overlap matrix $C_{ij} = \langle \mathbf{1}_i | \mathbf{1}_j \rangle$

a) Express $|1_i\rangle$ in terms of $|\sigma_i\rangle$ [this requires $P(x|i)$ and $\lambda(i,x)$]

b) Express the coefficients C_{ij} in terms of $\langle \sigma_i | \sigma_j \rangle$ → leading to $c = Qc$ with system matrix Q

c) Solve the constraint optimization problem

$$\text{argmin}_c \|c - Qc\|_2^2 \qquad \text{such that} \qquad C_{ij} = C_{ji} \wedge C_{ii} = 1$$

A global minimum must exist (not necessarily unique).

Otherwise, not even a perfect simulation is possible.

The proof is yet missing.

Algorithm

2. Perform a low-rank approximation of C

a) Fix the topological complexity d a priori

b) Perform a singular value decomposition: $C = V\,\Sigma\,W^{\dagger} = V\,\Sigma\,V^{\dagger}$

c) Shrink to rank d: $C^{(d)} = V\,\Sigma^{(d)}\,V^{\dagger}$

The topological complexity can be defined **a priori**.

The approximation is **optimal** due to the SVD.

Algorithm

3. Derive quantum memory states $|\boldsymbol{\sigma_i}\rangle$

a) Shrink to rank d: $C^{(d)} = V\,\Sigma^{(d)}\,V^{\dagger} = V\sqrt{\Sigma^{(d)}}\sqrt{\Sigma^{(d)}}V^{\dagger} = L^{\dagger}L$. [sort of Cholesky Decomp.]

b) Identify the quantum memory states $\left|\sigma_i^{(d)}\right\rangle$ as columns of $L^{\dagger}$

Due to construction, the states satisfy $C_{ij}^{(d)} = \left\langle 1_i^{(d)} \middle| 1_j^{(d)} \right\rangle = \left\langle \sigma_i^{(d)} \middle| \sigma_j^{(d)} \right\rangle$.

Interpretation: the approximate states are the exact states *to a slightly different process*.

Algorithm

4. Construct the unitary simulator U

a) Assemble the 1-step simulation matrix F with columns $F_i = |1_i\rangle$

b) Solve the constraint optimization problem

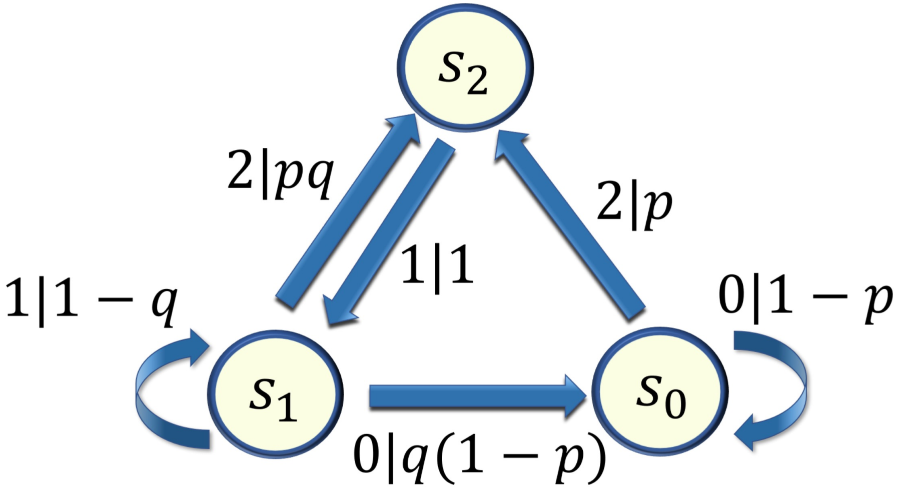
$$\underset{U}{\operatorname{argmin}} \left\| UL^\dagger - F \right\|_2^2 \qquad \text{such that} \qquad U^\dagger U = I$$

Due to construction, the Unitary satisfies $U \left|\sigma_i^{(d)}\right\rangle |0\rangle \approx \left|1_i^{(d)}\right\rangle$.

The approximation is **optimal** in the sense of a least-squares approximation.

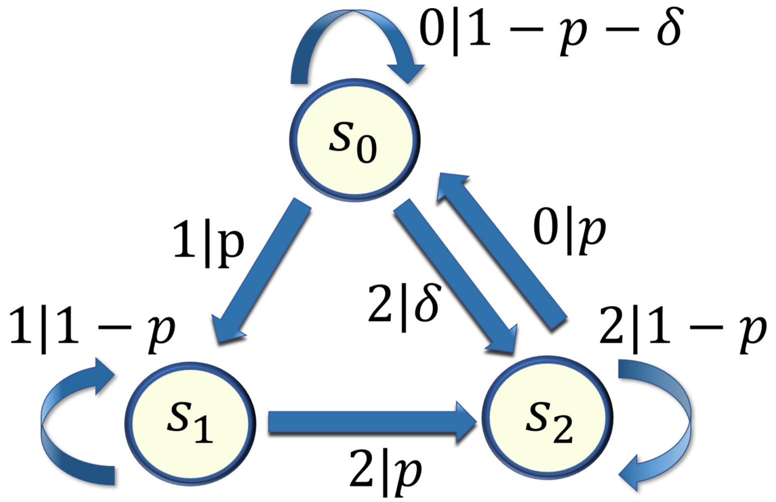
Results

Stochastic Processes



Asymmetric Process (p, q)

$d_c = 2 \quad d_q = 1$

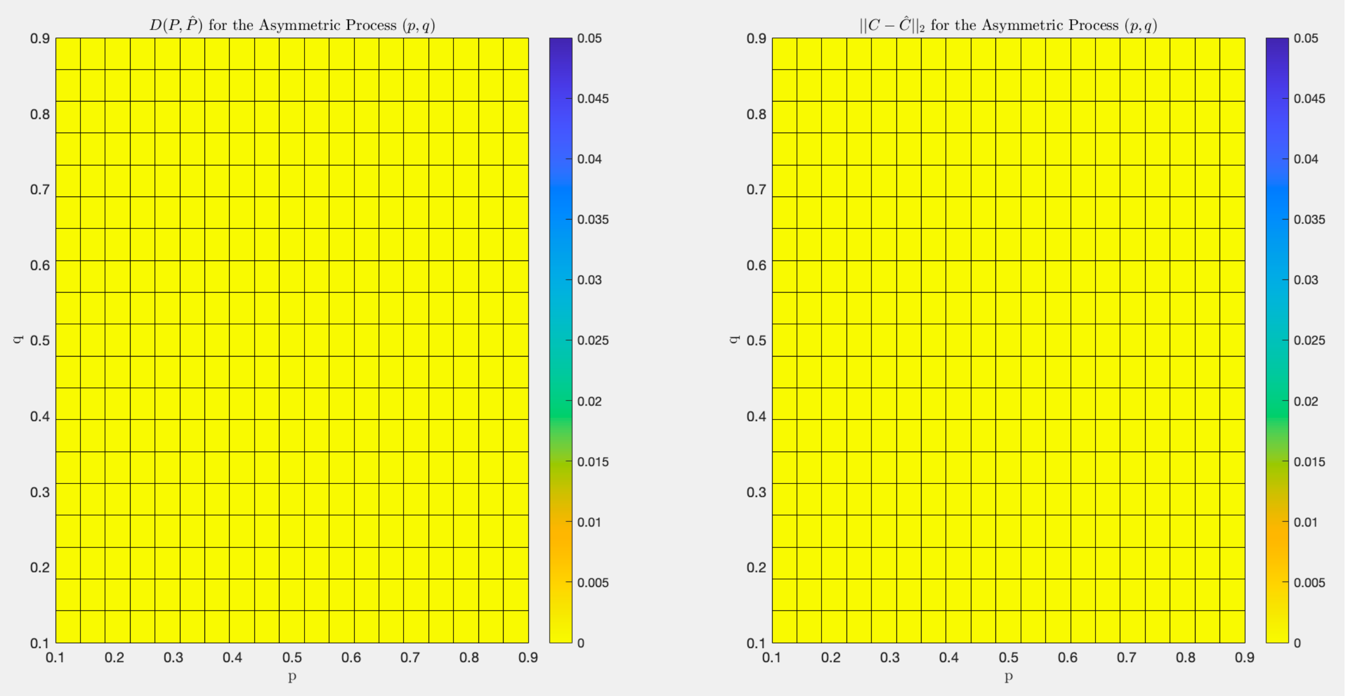


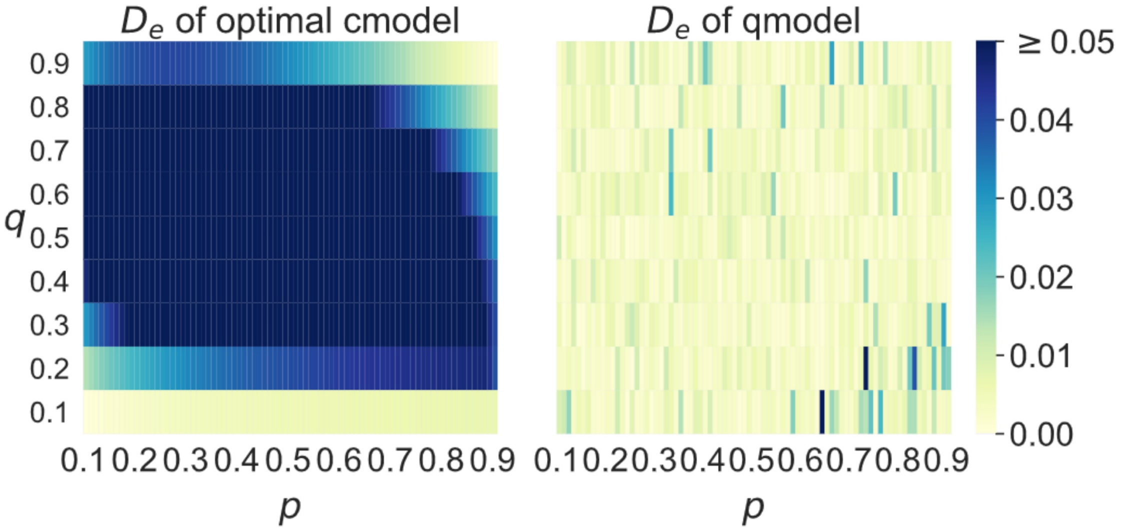
Quasi Cycle Process (p, δ)

$d_c = 2 \quad d_q = 2$

Yang et al., arXiv:2105.14434

Asymmetric Process (p, q)





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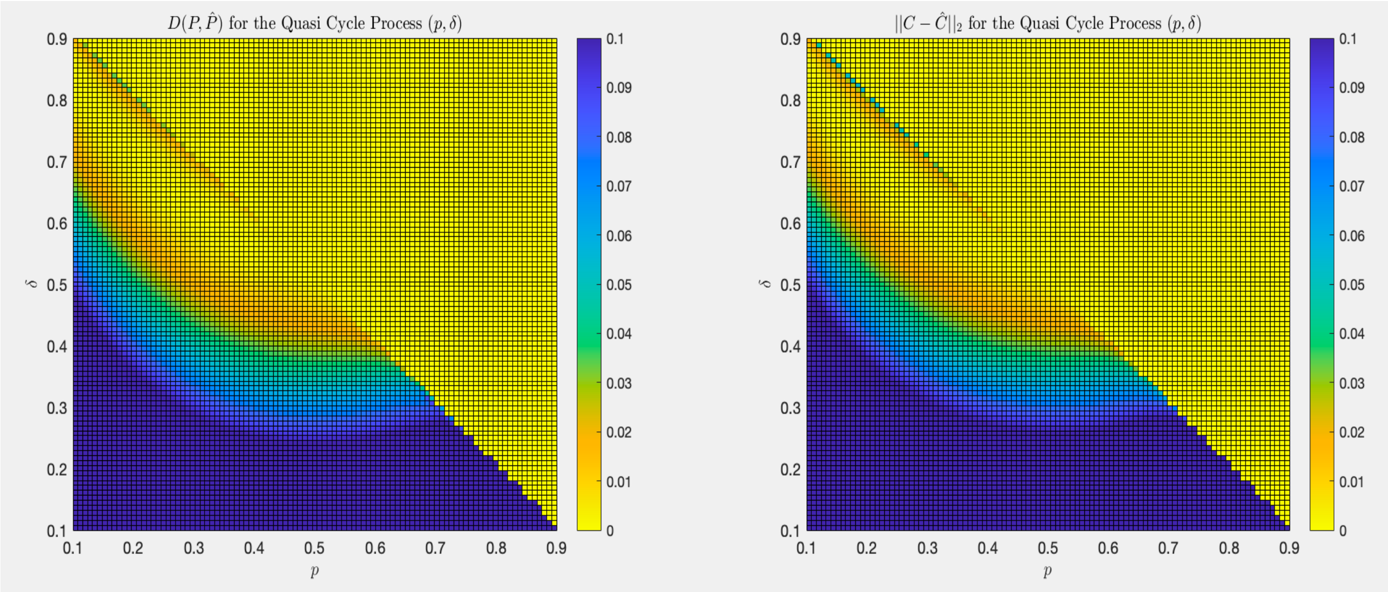
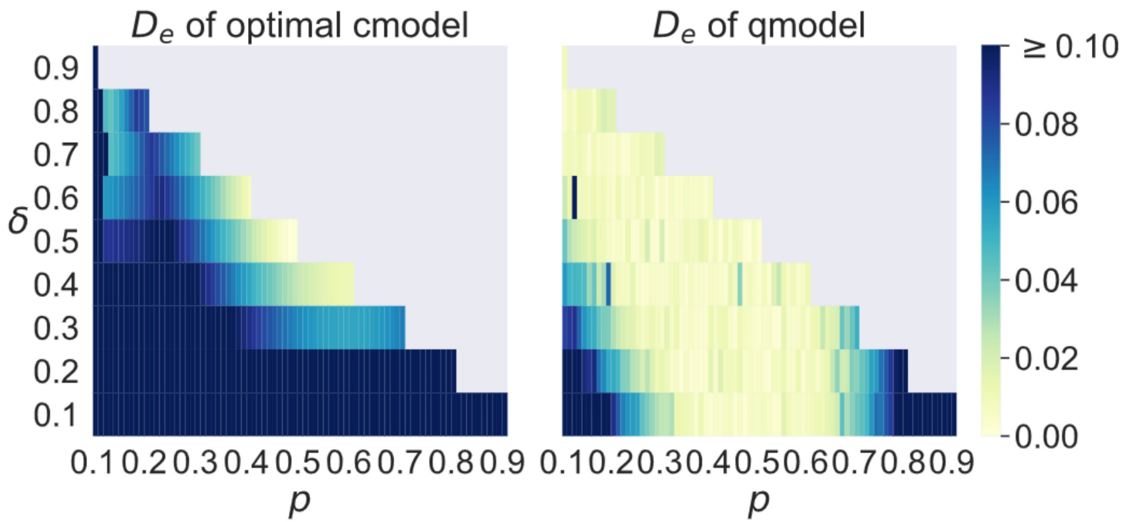




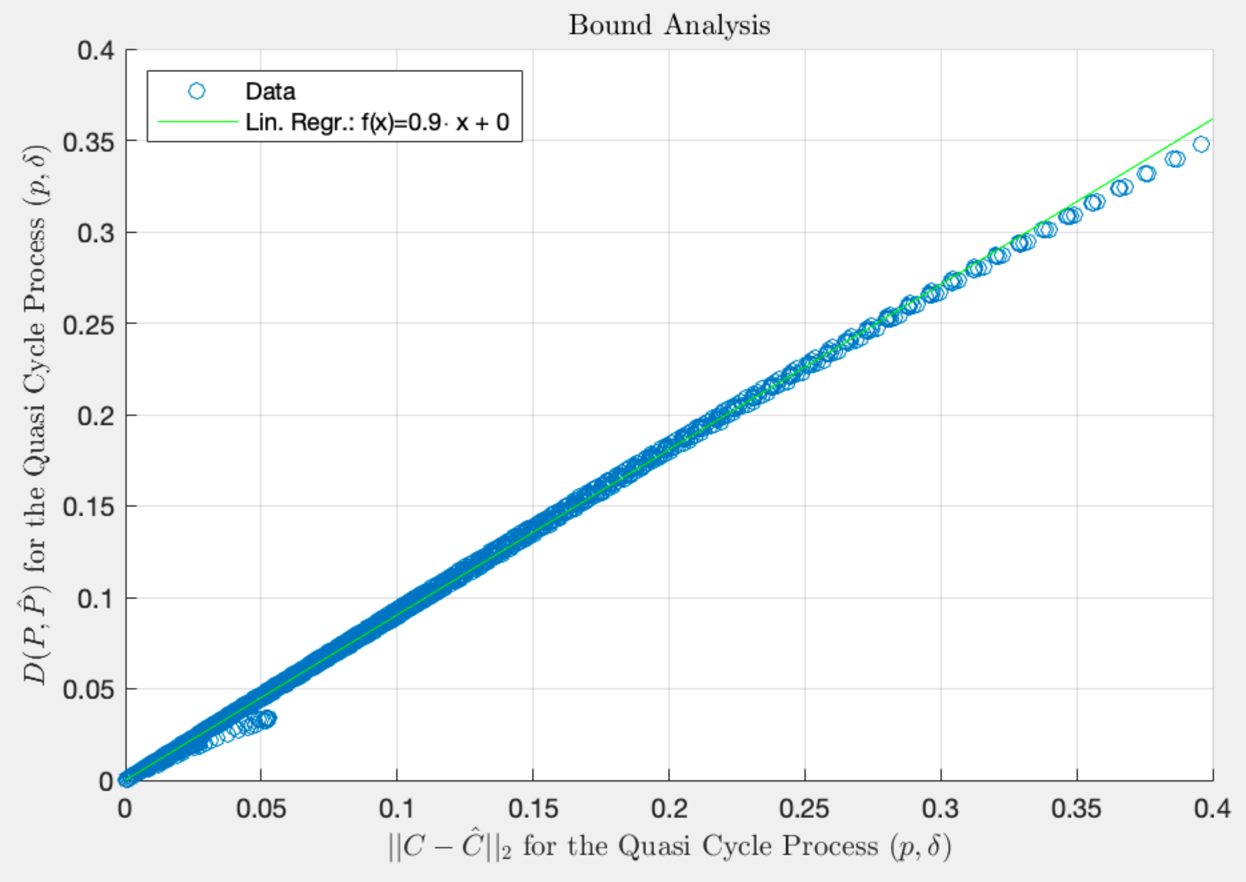
Yang et al., arXiv:2105.14434

Results

- The algorithm seems to work just fine.
- A "quantum advantage" exists for the approximate quantum models.
- By contrast, learned quantum models take complex phases into account.
- However, rigorous bounds seem possible, e.g.,

$$D\left(P, \hat{P}\right) \leq k(d) \cdot \left\|C - \hat{C}\right\|$$

Quasi Cycle Process (p, δ)



$$D(P, \hat{P}) \leq k(d) \cdot \|C - \hat{C}\|$$

Yang et al., arXiv:2105.14434

Benefits & Next Steps

- Derive lower bounds for the distortion
- Get insights on how to construct ansätze for the learning/data-driven case
- Description & interpretation for errors of approximate models
- The approach is not a black box

- Validate multiple time steps
- Rigorously proof some of the claimed statements
- Derive bounds

Yang et al., arXiv:2105.14434

Thanks!

Let’s discuss!