University of Stuttgart
Institute for Computational Physics

Freie Universität Berlin

SimTech

Simulating Stochastic Processes with Variational Quantum Circuits

Daniel Fink

Master Thesis

-

Presentation

February 14th, 2022

Advisors

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- Free University of Berlin
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  - Dr. Nora Tischler
  - Dr. Ryan Sweke
  - M.Sc. Paul Fährmann

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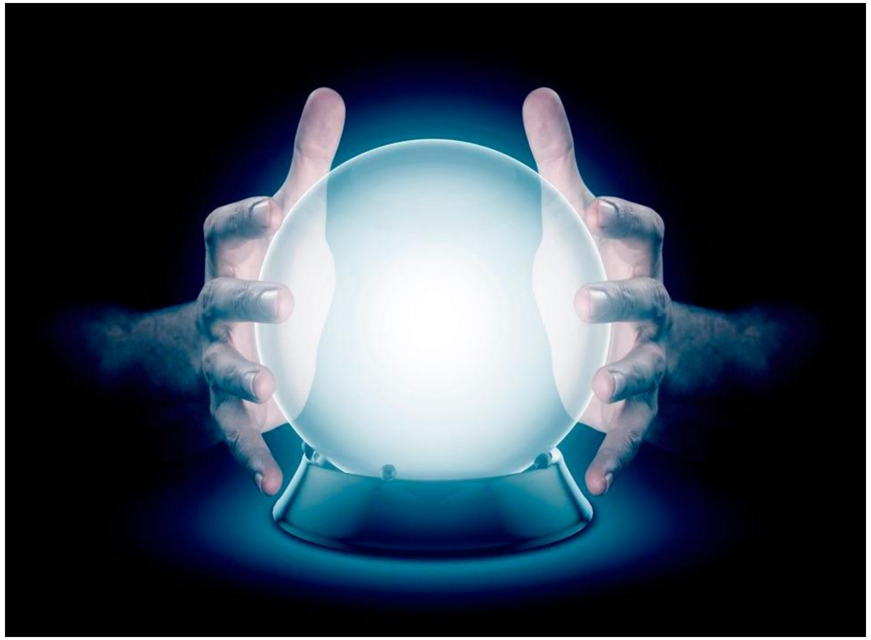
Motivation

Can we predict the future based on past observations?



Motivation

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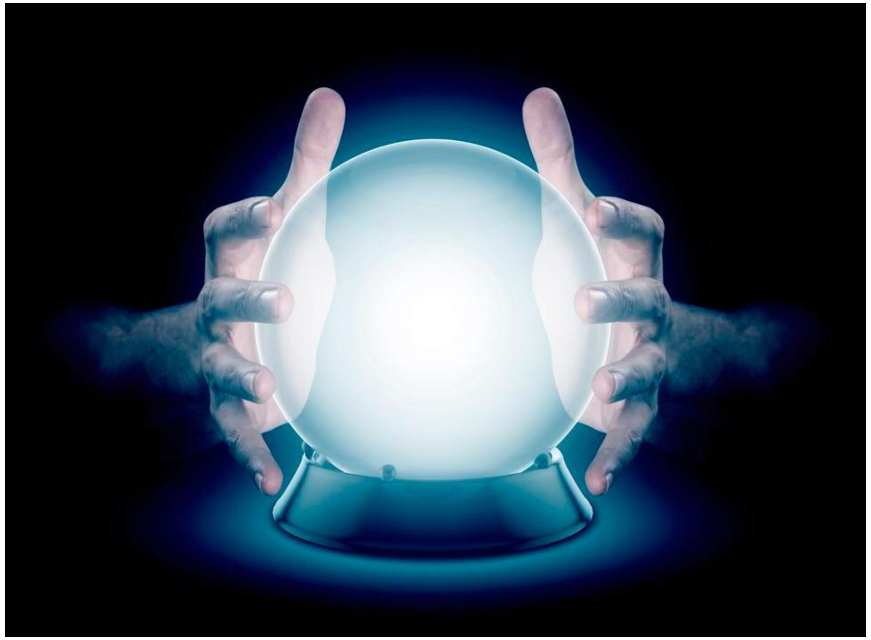


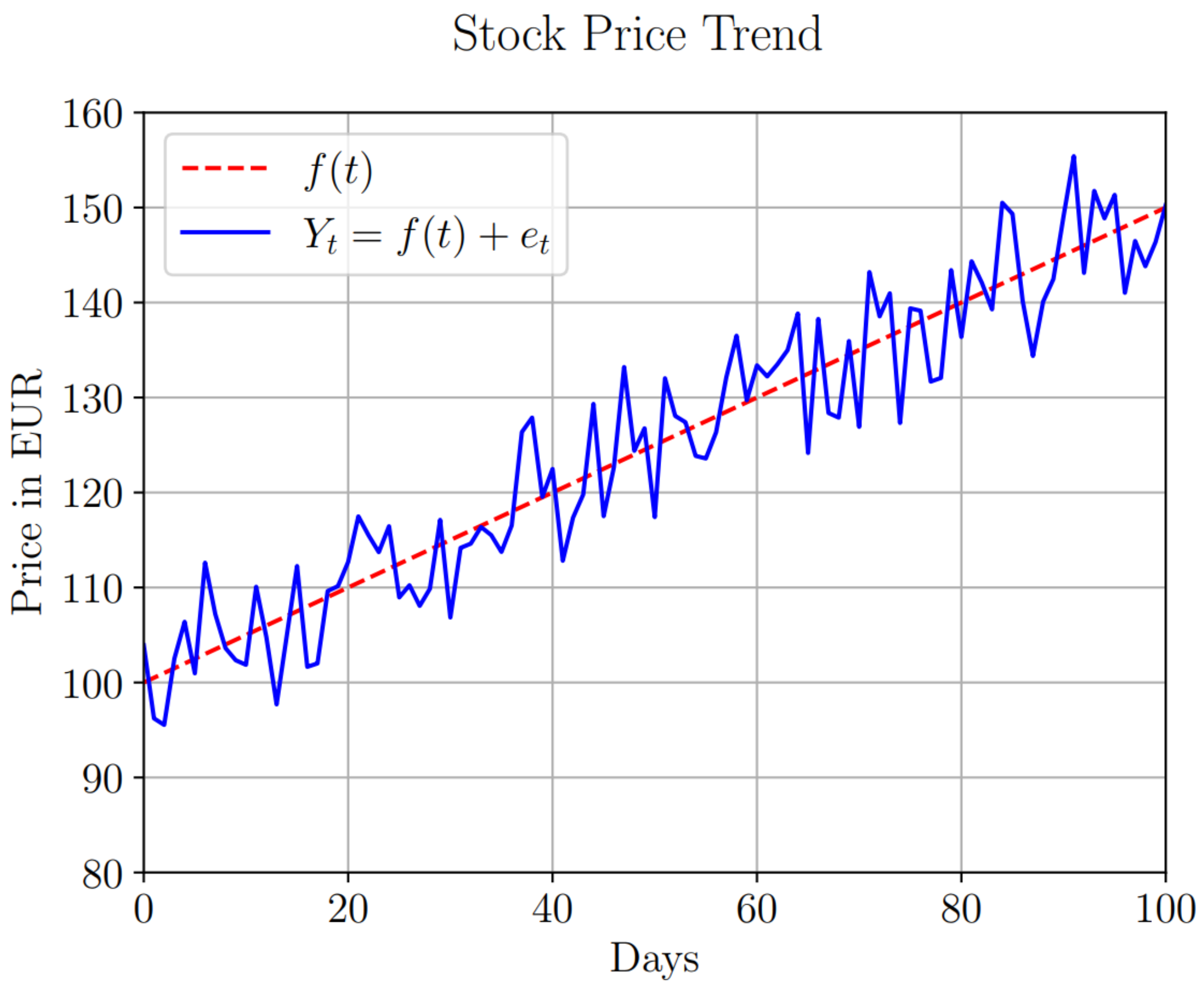
Simulations → show possible futures

Motivation

Assume linear trend $f(t)$

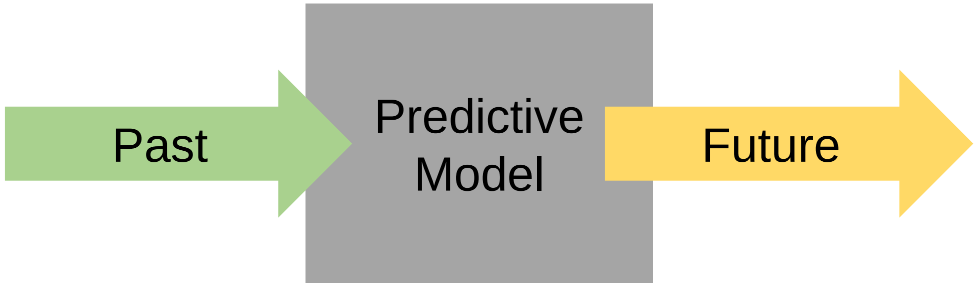
Add some noise e_t

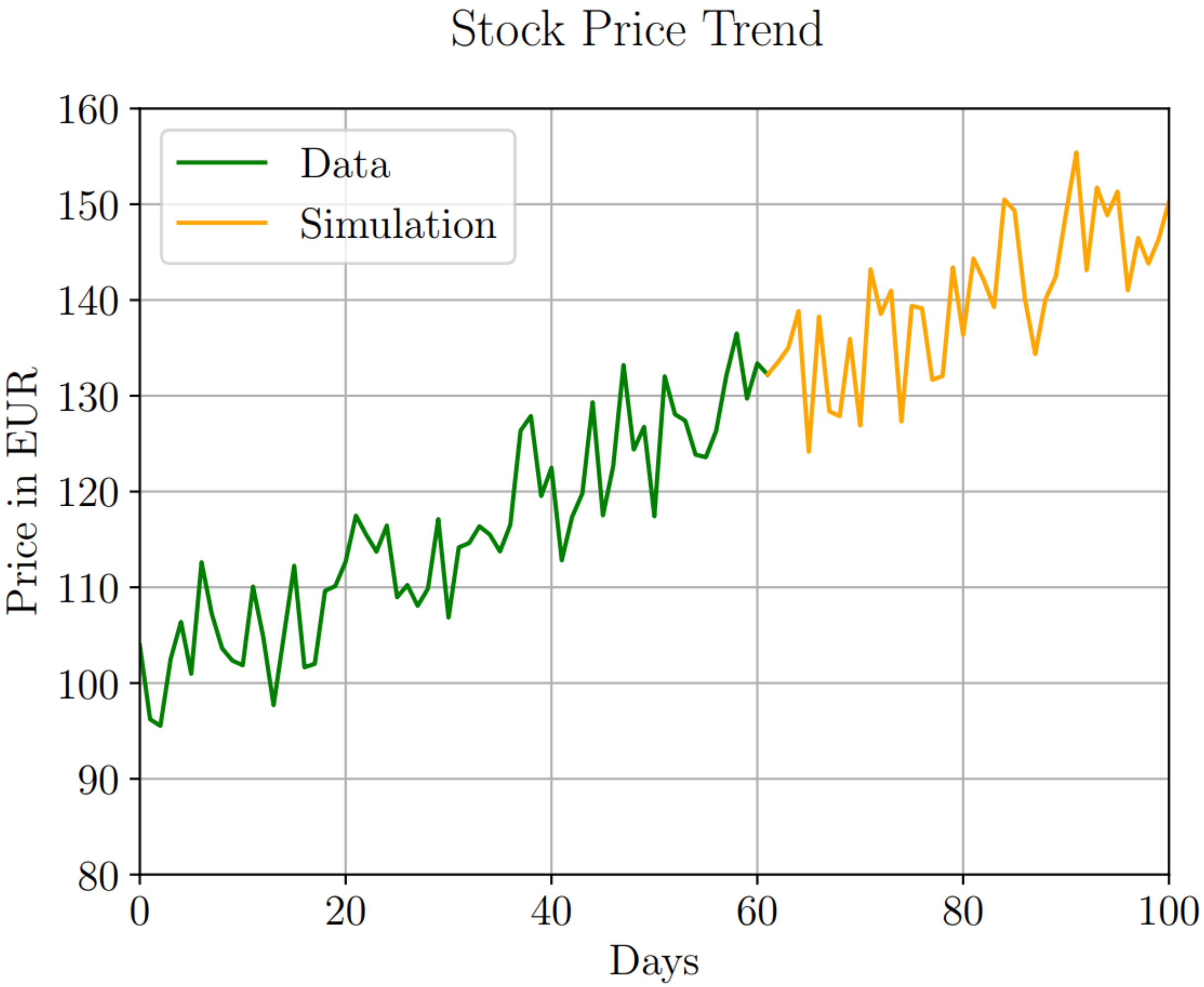
→ e_t is a stochastic process



Motivation

Assume data drawn
by a stochastic process





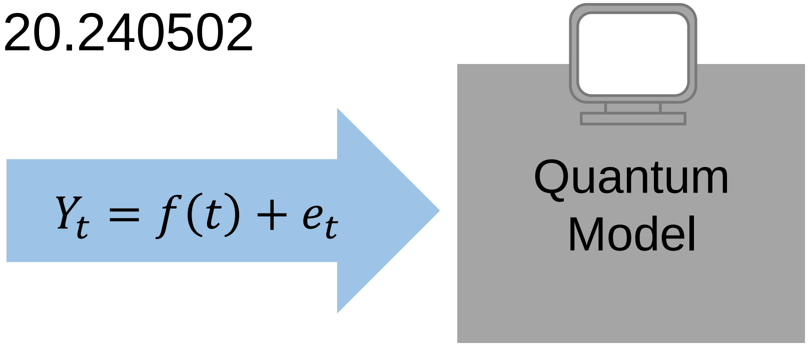
Motivation

Classical Models $\leq$ Quantum Models

How to get a quantum model?

Motivation

- Classical description of the process → q–simulator
    - Binder et al., 10.1103/PhysRevLett.120.240502



Motivation

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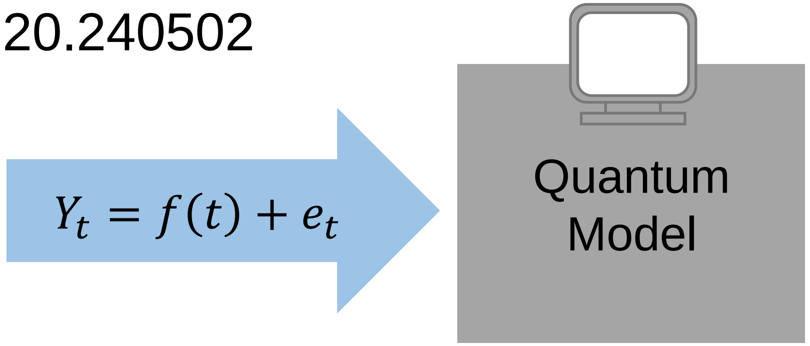
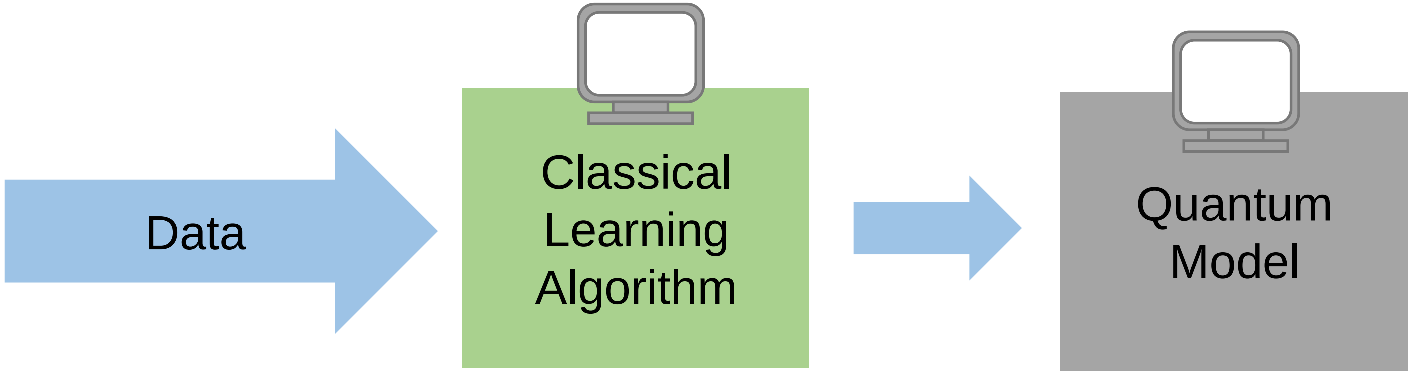


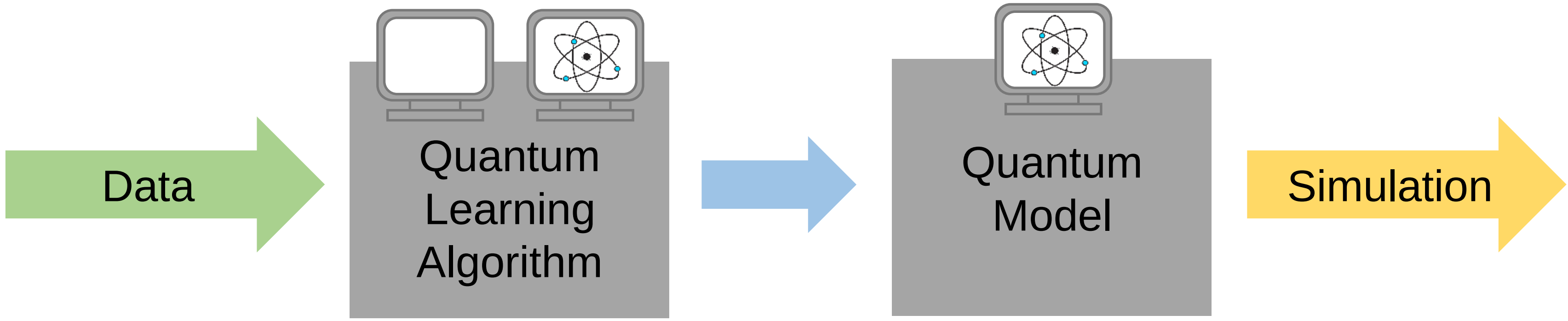
- Data from the process → classical discovery algorithm
  - Yang et al., arXiv:2105.14434



Motivation

Goal

Develop a quantum learning algorithm for predictive models, which uses only data as input.



Content

- Stochastic Processes
- ϵ–machine
- Quantum Circuits
- q–simulator
- Quantum Learning Algorithm
- Results
- Conclusion

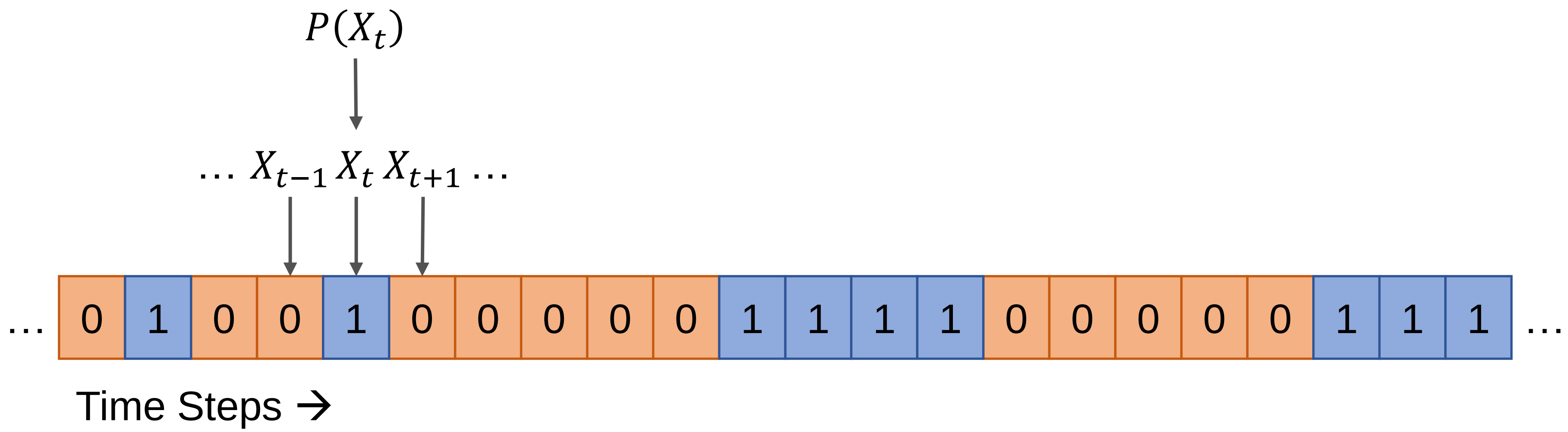
Stochastic Processes

Stochastic Processes

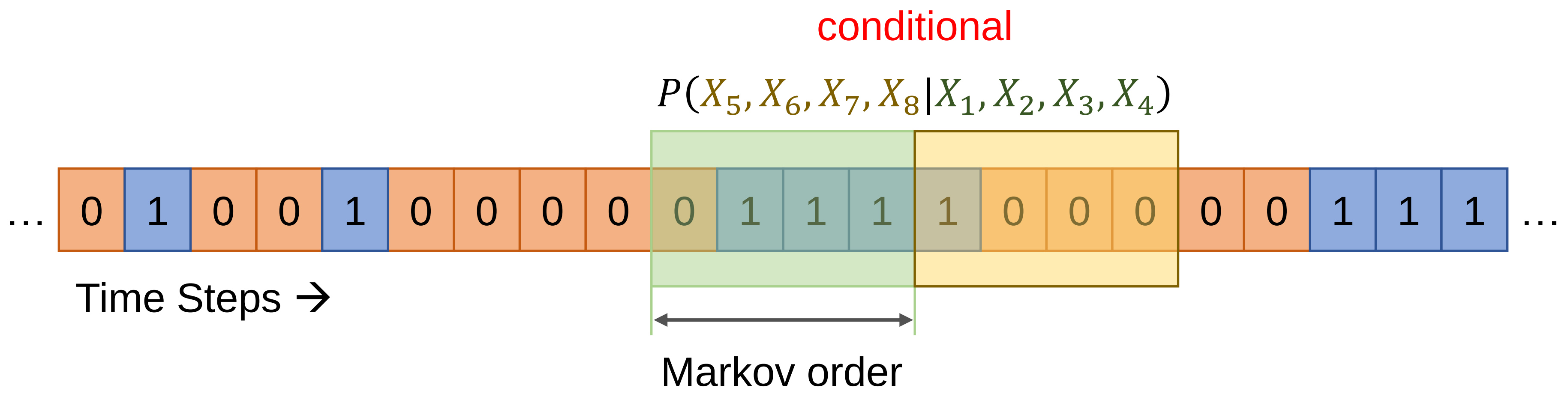
… | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 1 | …

Time Steps →

Stochastic Processes

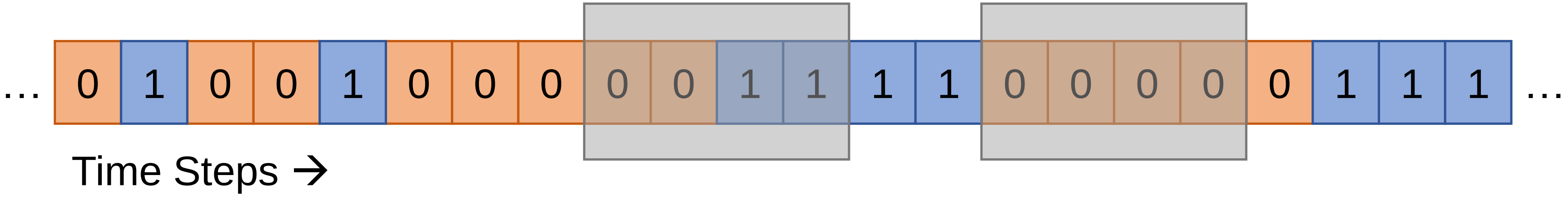


Stochastic Processes

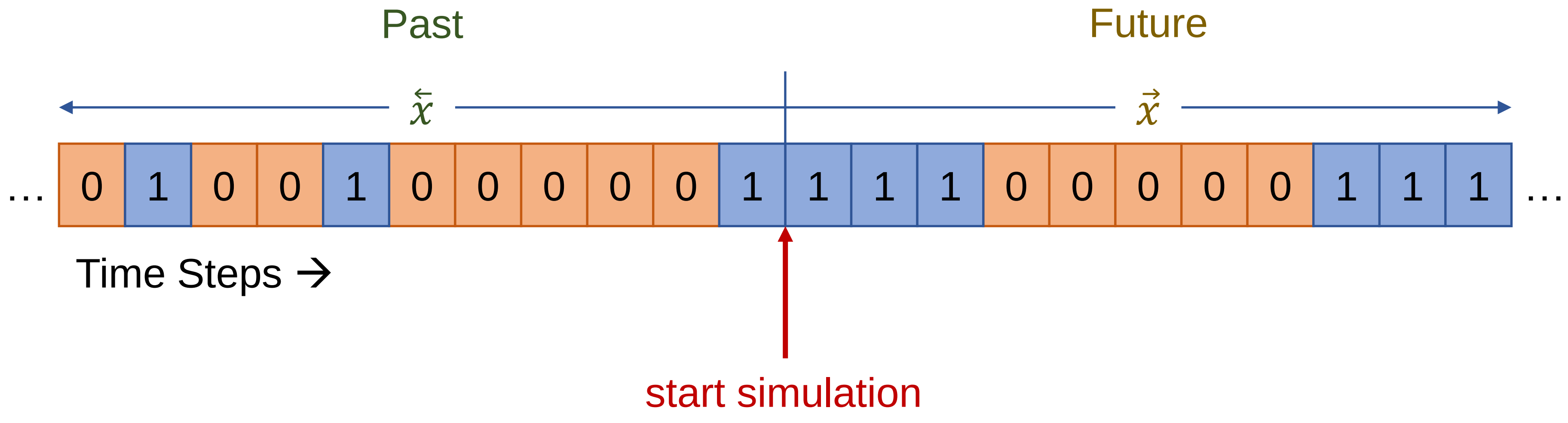


stationary

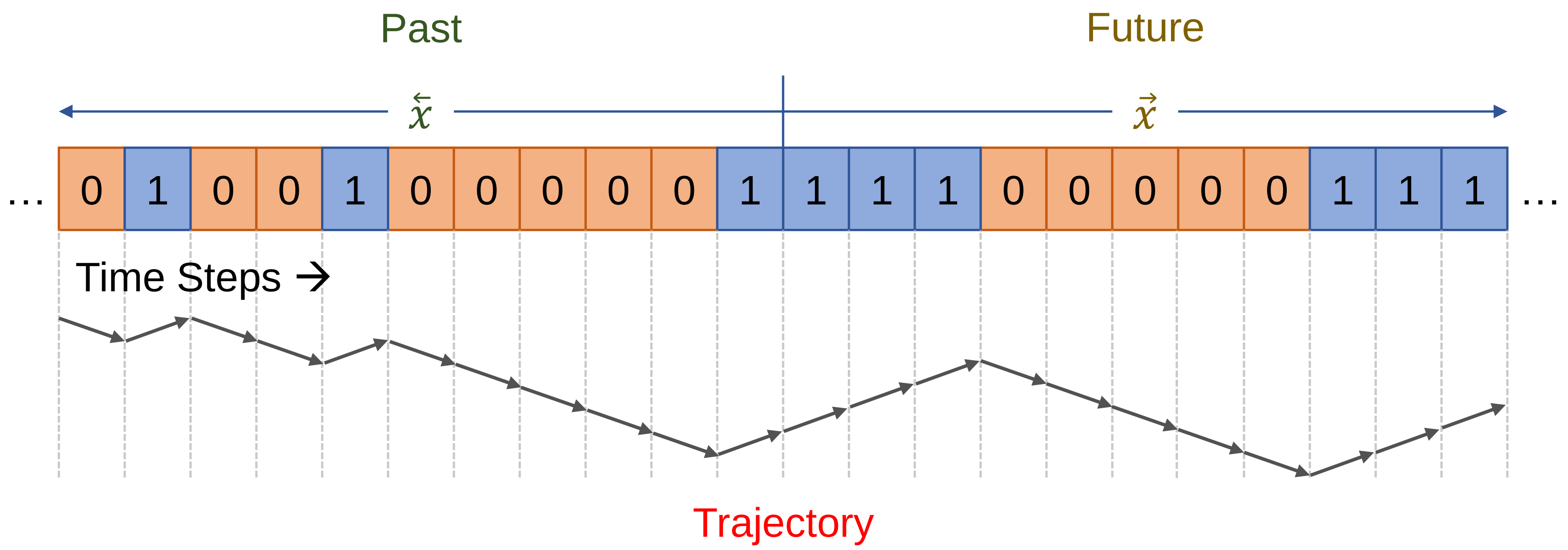
$$P(X_1, X_2, X_3, X_4) \quad = \quad P(X_5, X_6, X_7, X_8)$$



Stochastic Processes

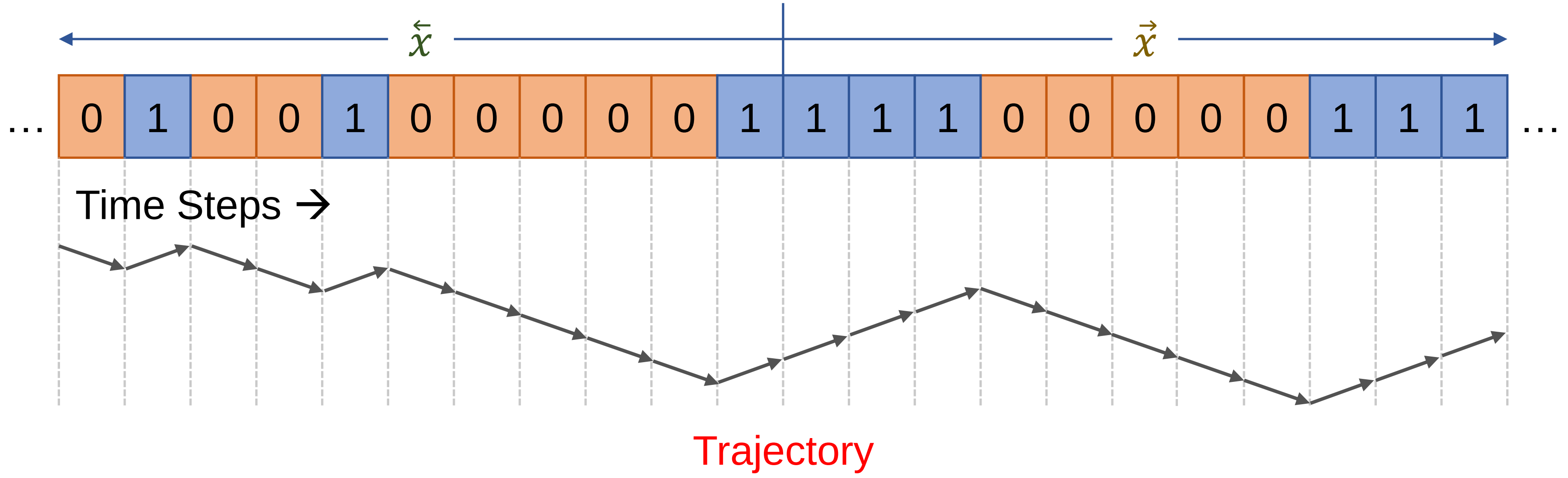


Stochastic Processes



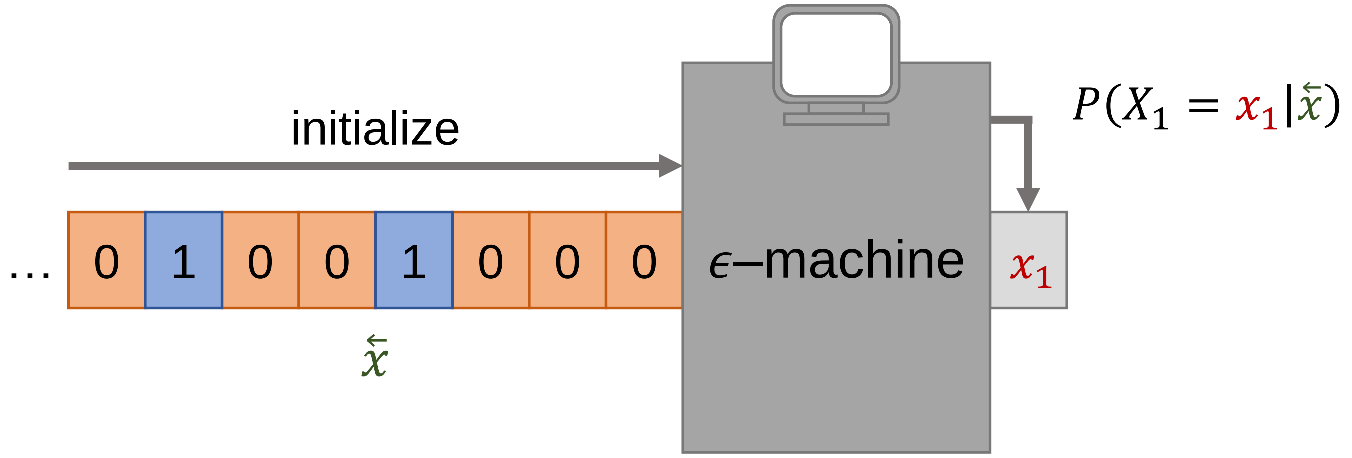
Stochastic Processes

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



ϵ–machine

ϵ–machine



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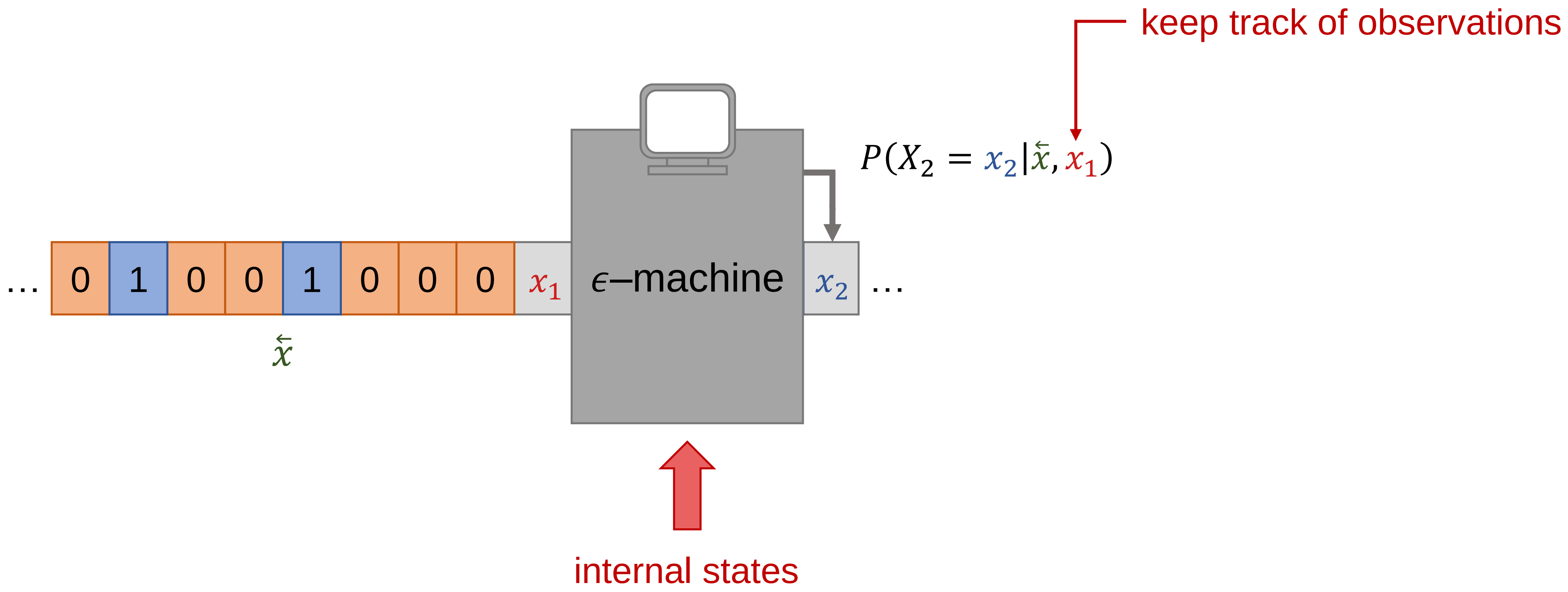
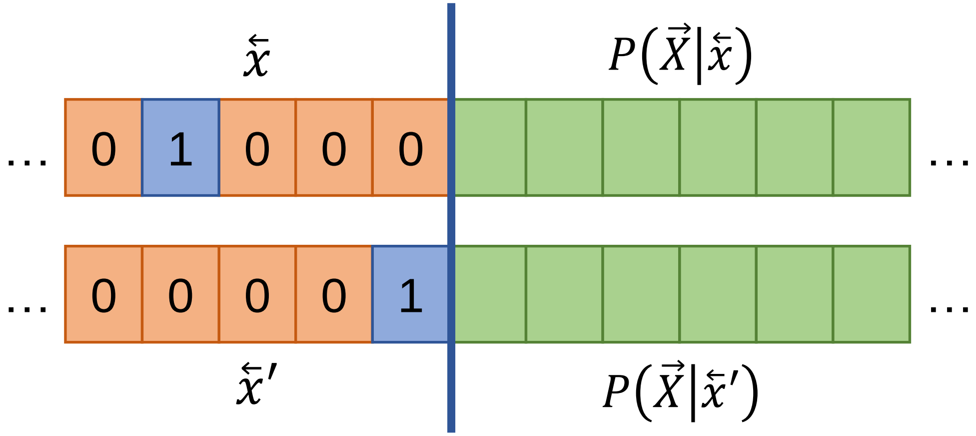
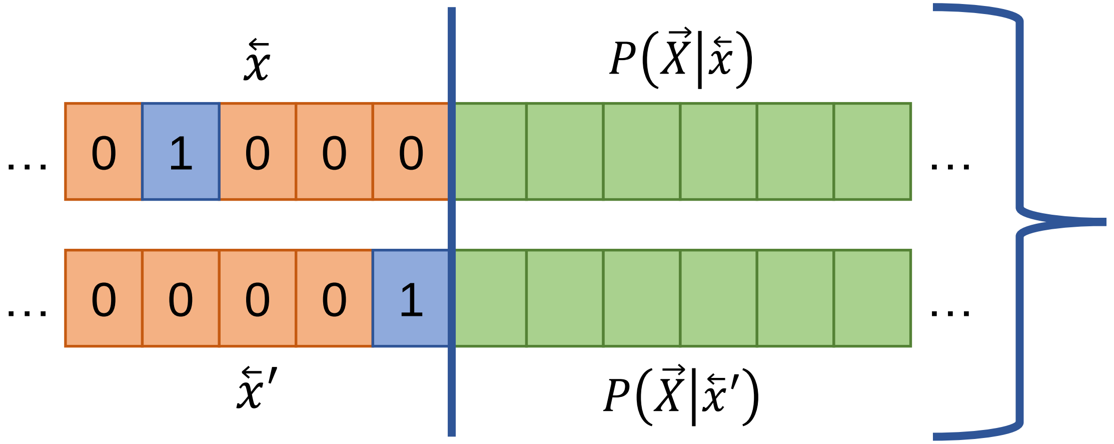


ϵ–machine

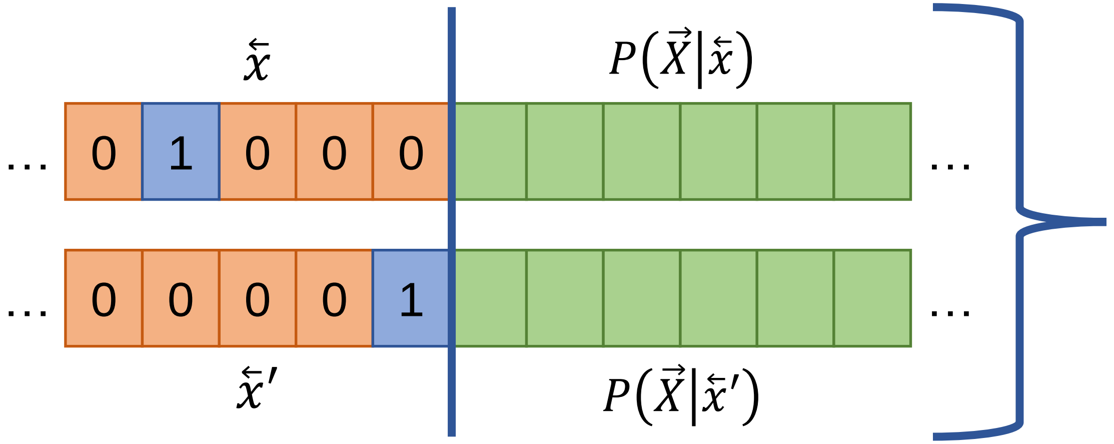


ϵ–machine



$$\overleftarrow{x} \sim \overleftarrow{x}' \iff P(\overrightarrow{X}|\overleftarrow{x}) = P(\overrightarrow{X}|\overleftarrow{x}')$$

ϵ–machine



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

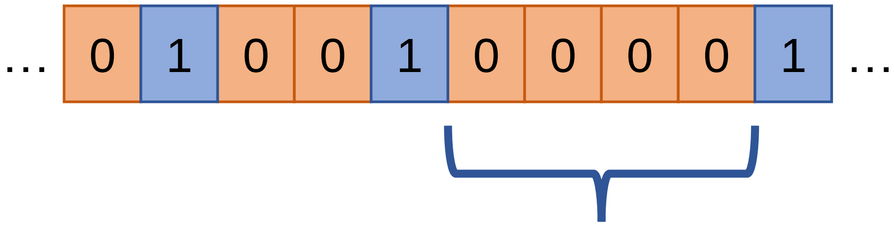
→ causal sates $\{S_i\}_{i=1}^{N}$ (minimal)

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

Classical Topological Complexity: $d_c = \log_2 N$

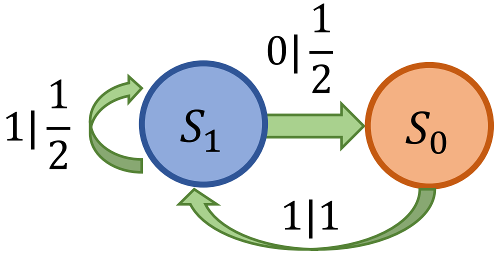
Example

Period-N Uniform Renewal Process



$\sim U(0, N-1)$

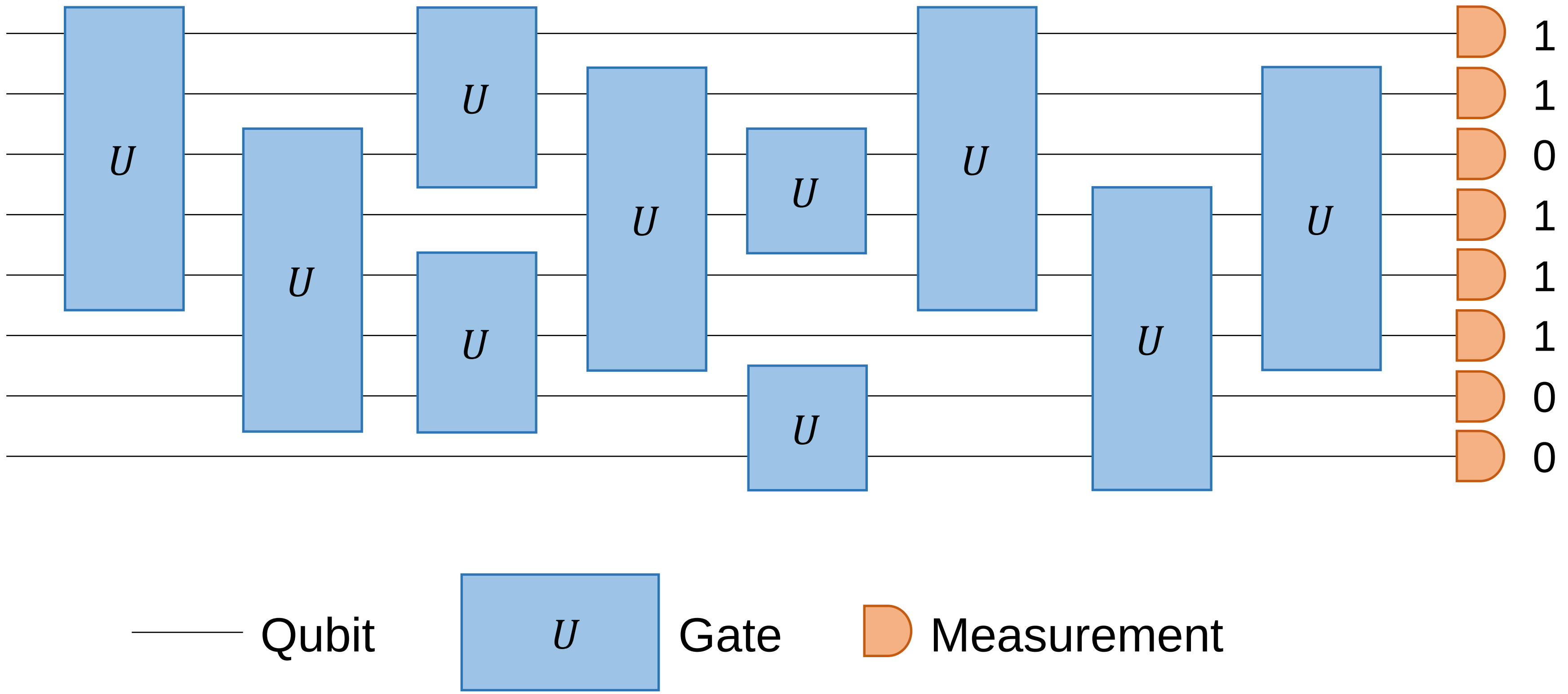
Period = 2



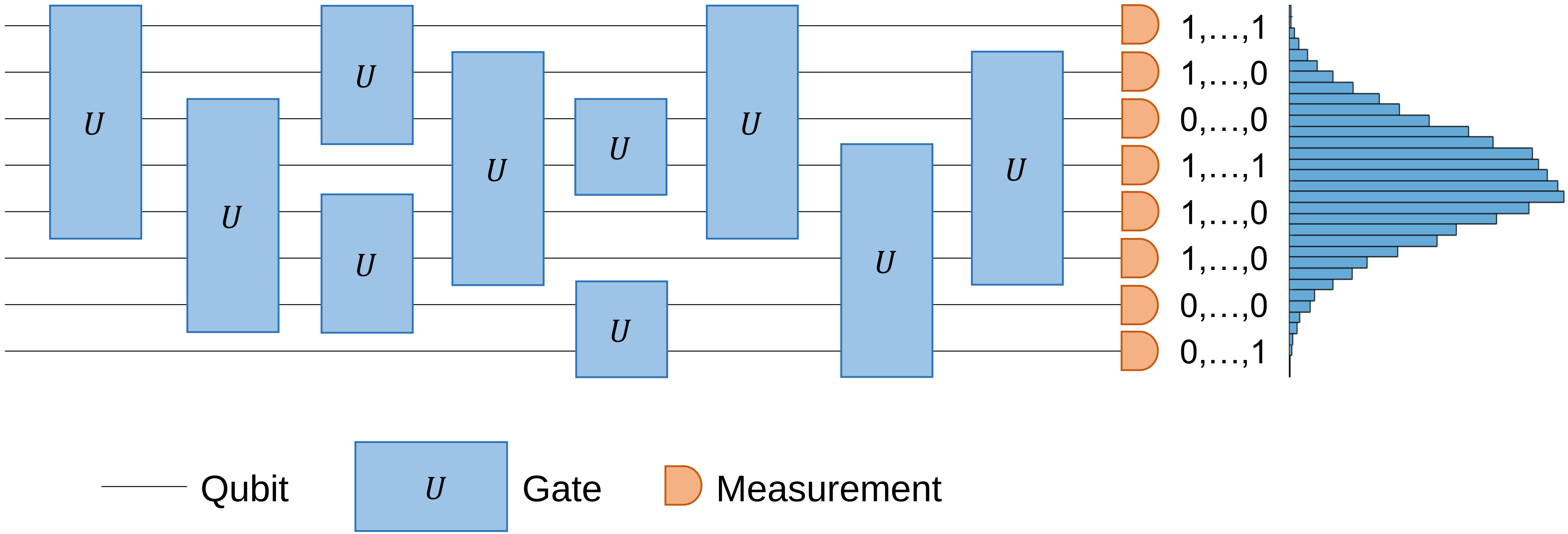
ϵ-machine

Quantum Circuits

Quantum Circuits

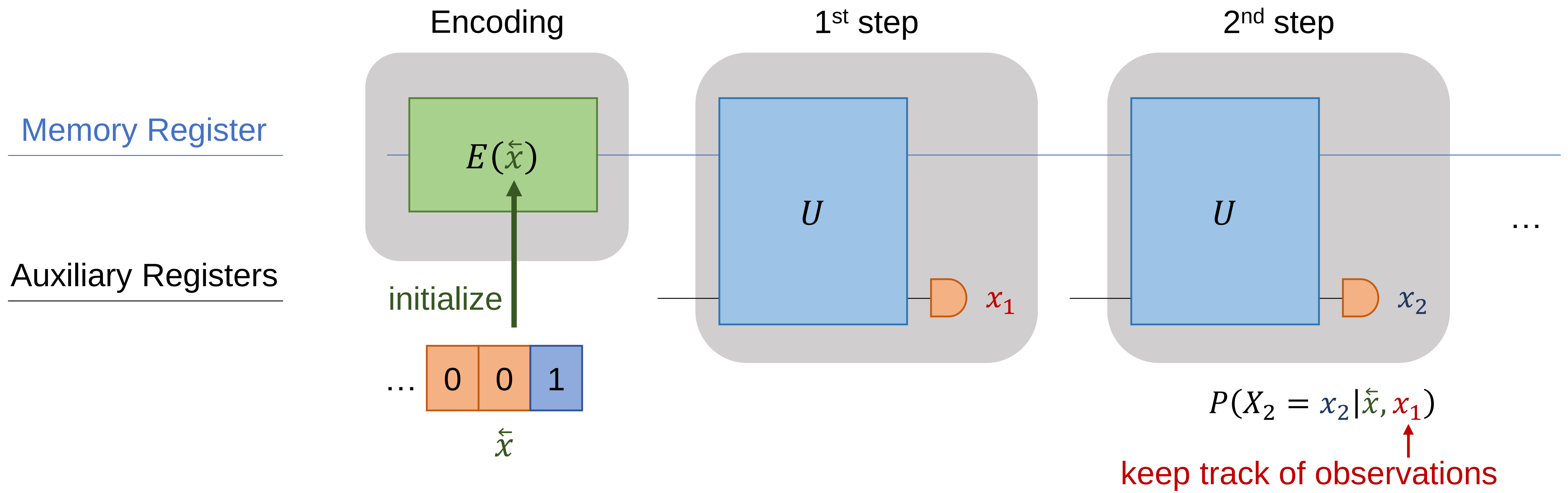


Quantum Circuits



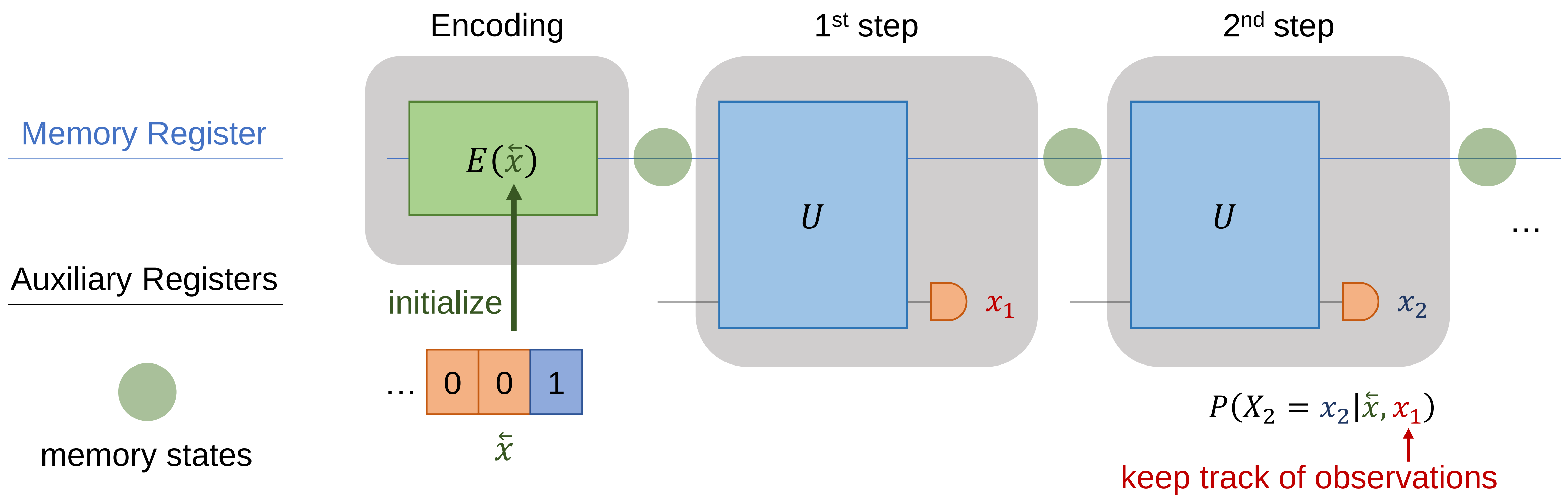
q–simulator

q–simulator



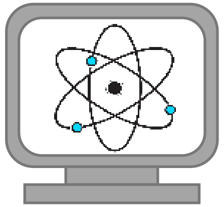
Encoding
1st step
2nd step
Memory Register
Auxiliary Registers
$E(\overleftarrow{x})$
initialize
U
U
x_1
x_2
…
… 0 0 1
$\overleftarrow{x}$
$P(X_2 = x_2 | \overleftarrow{x}, x_1)$
keep track of observations

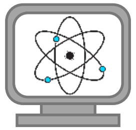
q–simulator



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

Advantage

In general:  $d_q \leq d_c$ 

For some processes:  $d_q < d_c$ 

Thompson et al., 10.1103/PhysRevX.8.031013

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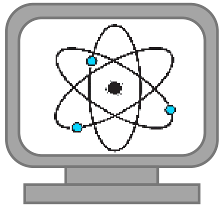
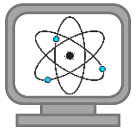
In general:  $d_q \leq d_c$ 

For some processes:  $d_q < d_c$ 

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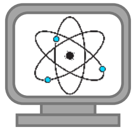
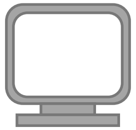
Approximate models:  $\hat{d}_q = \hat{d}_c$ 

Q-Models can have better accuracy
Yang et al., arXiv:2105.14434

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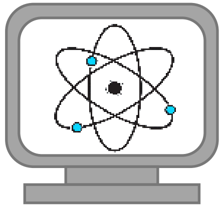
In general:  $d_q \leq d_c$ 

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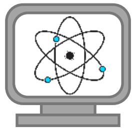
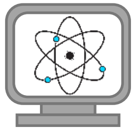
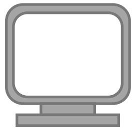
For some processes:  $d_q < d_c$ 

Approximate models:  $\hat{d}_q = \hat{d}_c$ 

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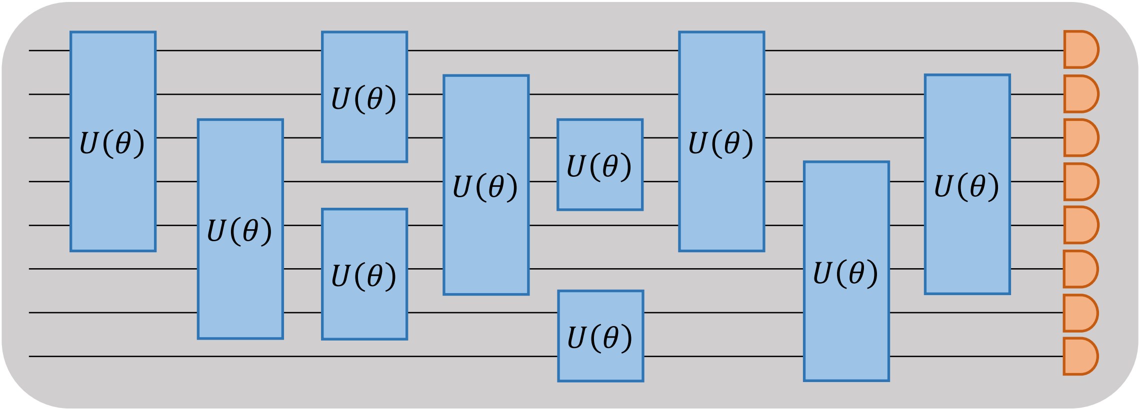
How to get a **quantum representation** of a quantum model?

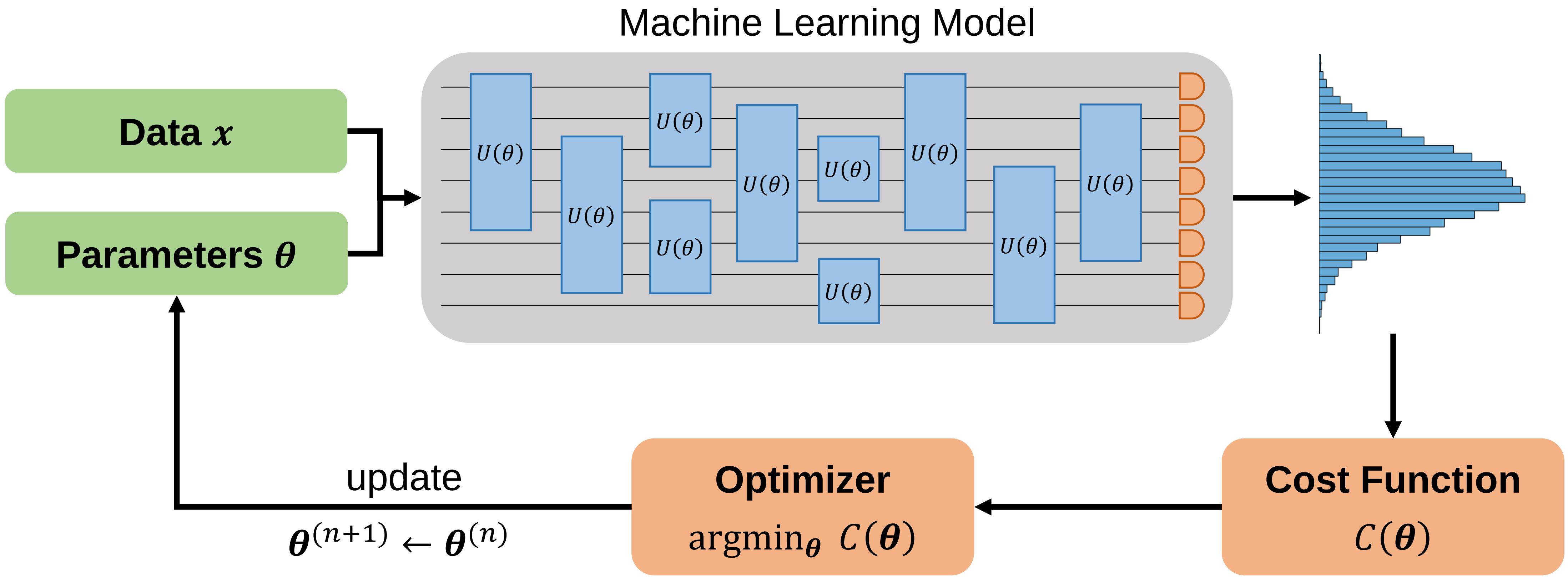
Variational Quantum Circuits

Variational Quantum Circuits

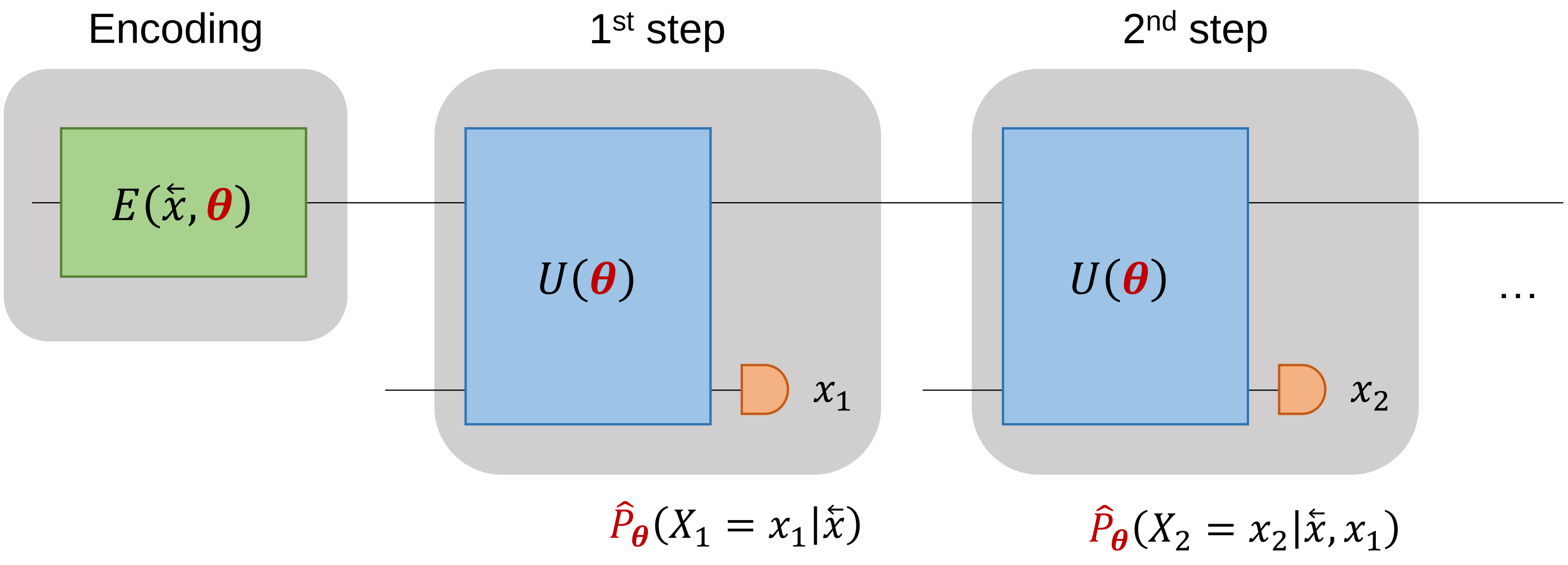
Machine Learning Model



Variational Quantum Algorithms



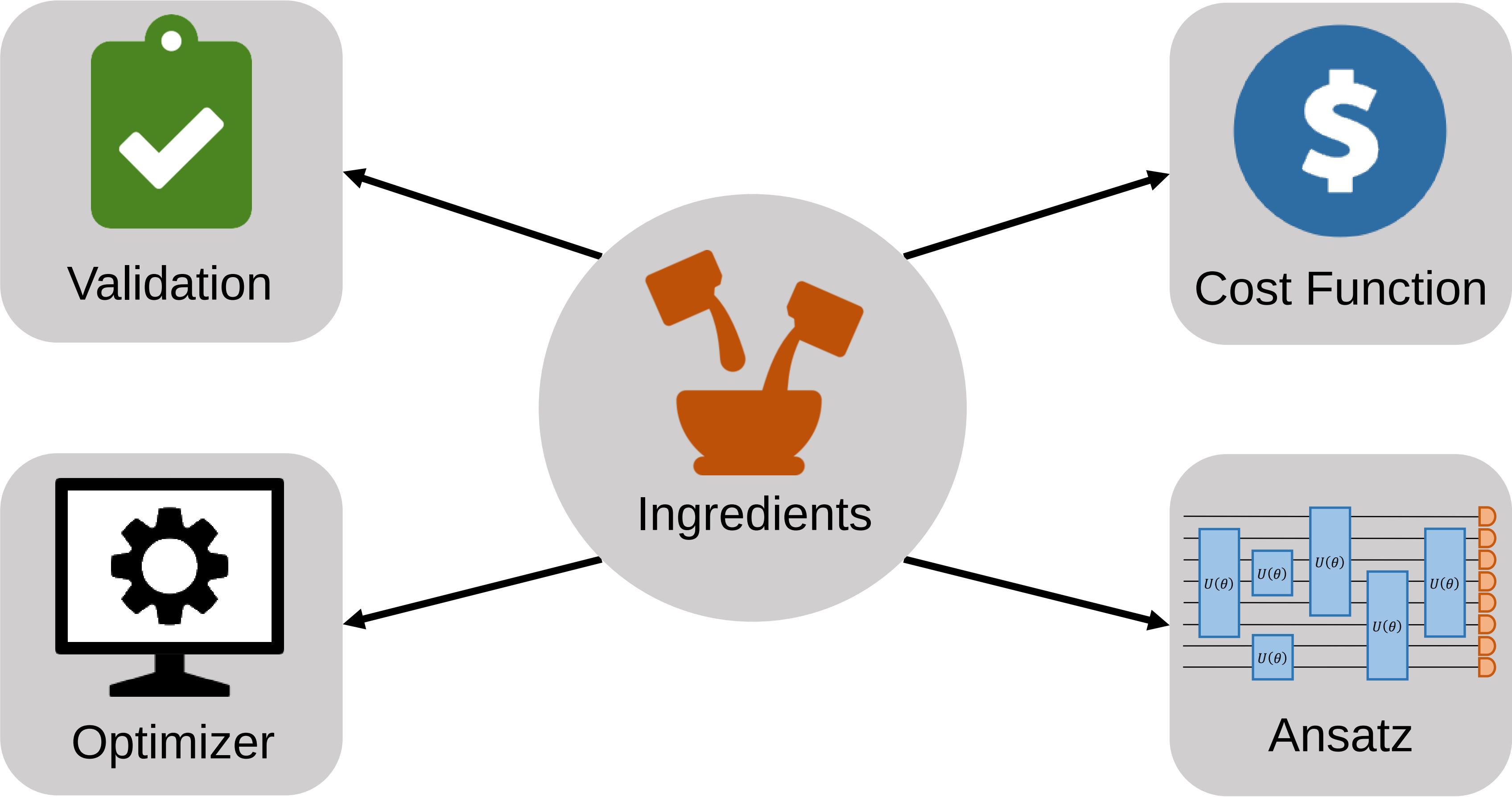
Idea



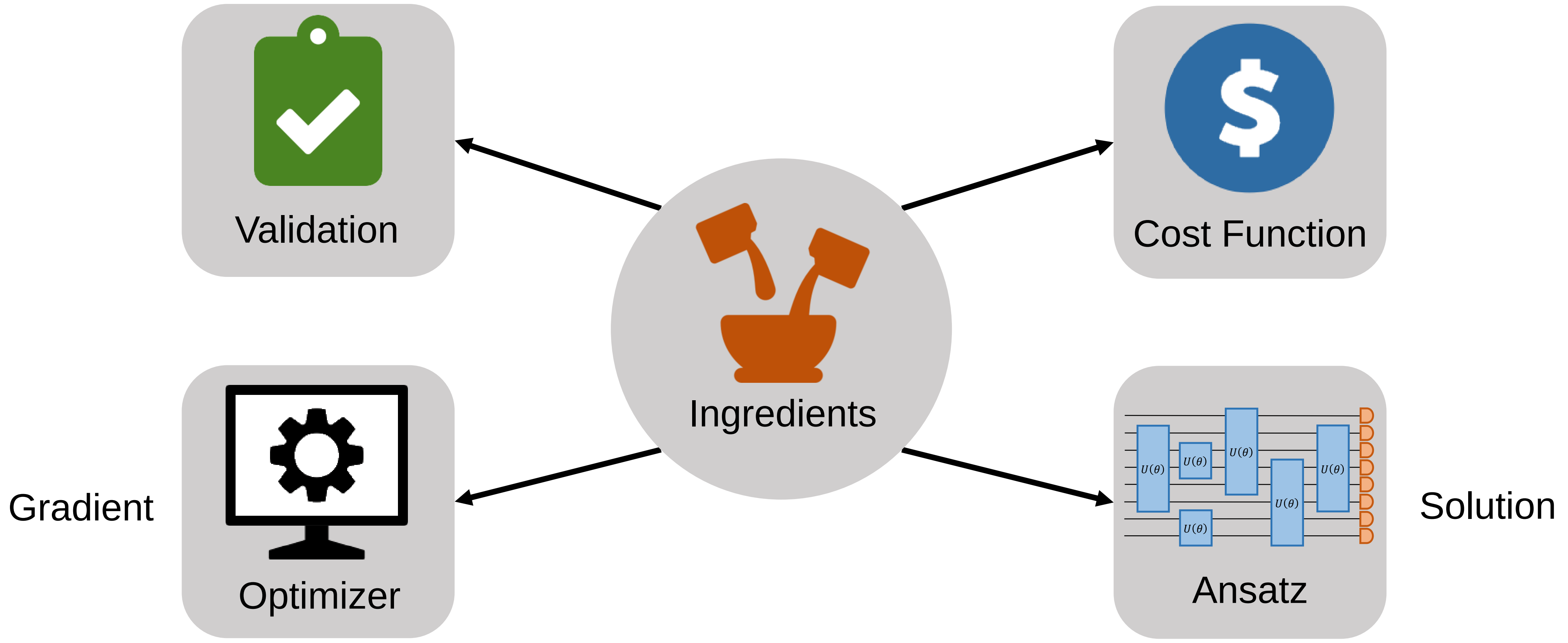
Approximate P → $\left| P - \hat{P}_{\boldsymbol{\theta}} \right| < \delta$

Quantum Learning Algorithm

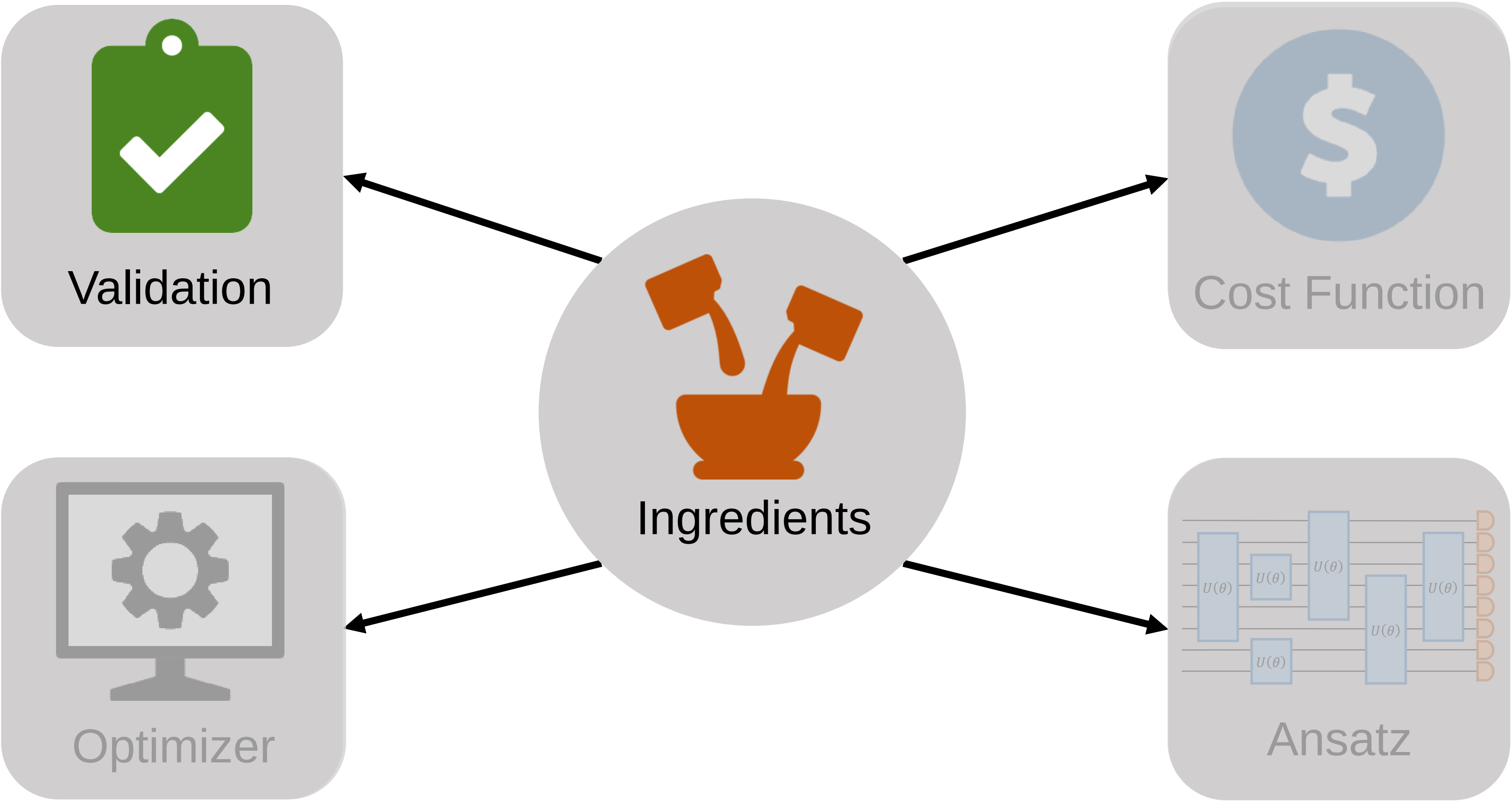
Quantum Learning Algorithm



Quantum Learning Algorithm



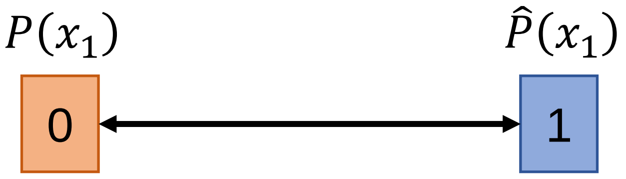
Quantum Learning Algorithm



Validation

Kullback-Leibler divergence:
(KL)

$$D_{KL}(P, \hat{P}) = \sum_x P(x) \log_2 \frac{P(x)}{\hat{P}(x)}$$



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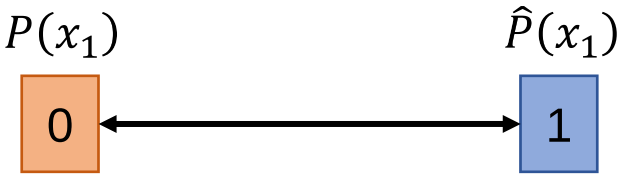


mean over time steps

average over pasts

Validation

Kullback-Leibler divergence:
(KL)

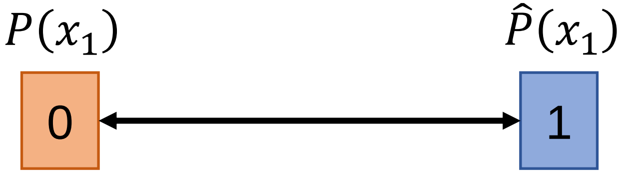
$$D_{KL}(P,\hat{P}) = \sum_x P(x) \log_2 \frac{P(x)}{\hat{P}(x)}$$

mean over time steps

average over pasts

Total Variation Distance:
(TV)

$$D_{TV}(P,\hat{P}) = \frac{1}{2}\sum_x \left|P(x) - \hat{P}(x)\right|$$



Validation

Kullback-Leibler divergence: (KL)

$$D_{KL}(P,\hat{P}) = \sum_x P(x)\log_2\frac{P(x)}{\hat{P}(x)}$$

$P(x_1)$ 0 ⟷ 1 $\hat{P}(x_1)$

mean over time steps

average over pasts

Total Variation Distance: (TV)

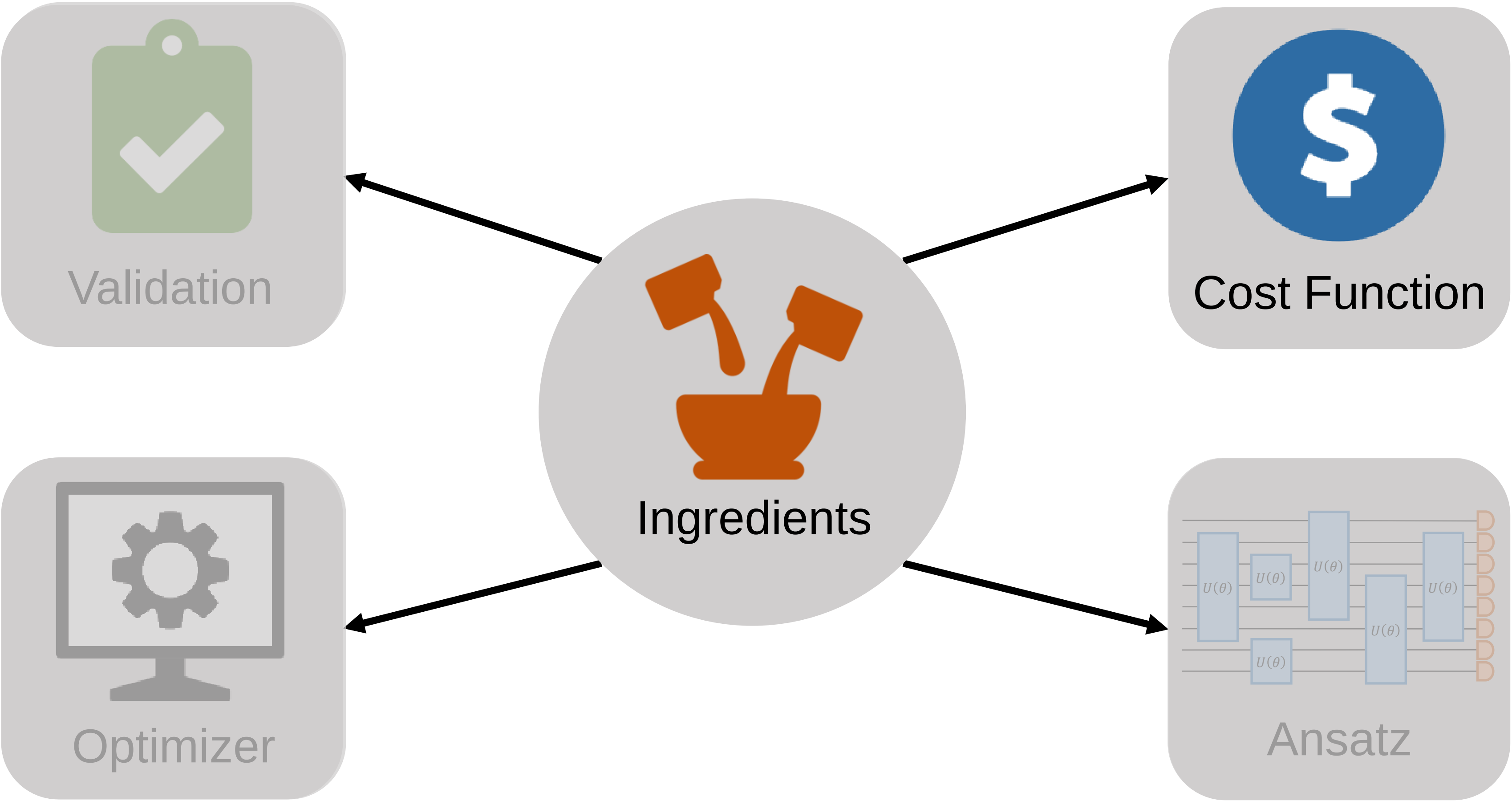
$$D_{TV}(P,\hat{P}) = \frac{1}{2}\sum_x \left|P(x)-\hat{P}(x)\right|$$

$P(x_1)$ 0 ⟷ 1 $\hat{P}(x_1)$

sum up time steps

sum up pasts

Quantum Learning Algorithm



Cost Function

Ideally, use validation metric: $$D_{KL}(P, \hat{P}) = \sum_x P(x) \log_2 \frac{P(x)}{\hat{P}(x)}$$

Cost Function

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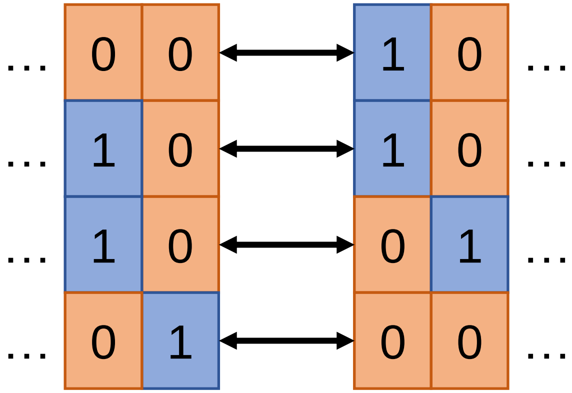
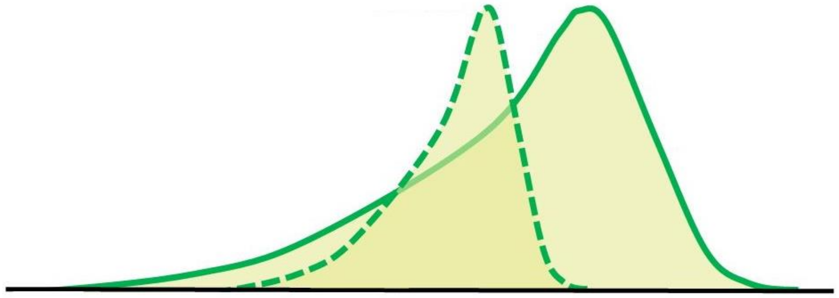
unknown

inefficient

Cost Function

Maximum Mean Discrepancy:
(MMD)

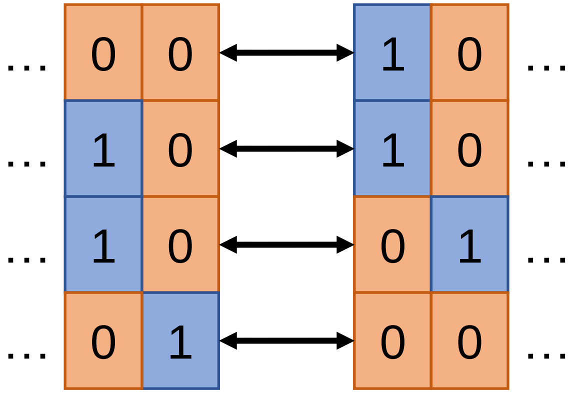


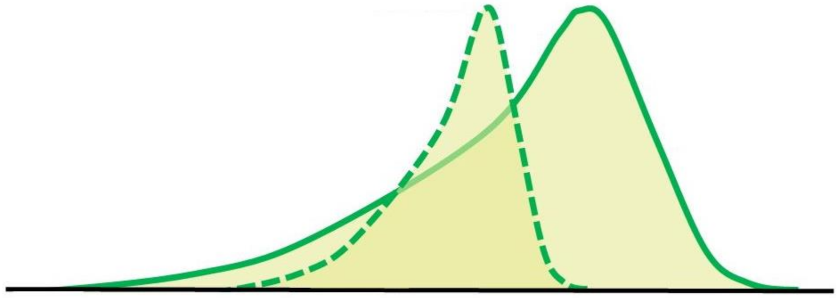


$$\mathrm{MMD}\left[P, \hat{P}\right] = 0 \iff P = \hat{P}$$

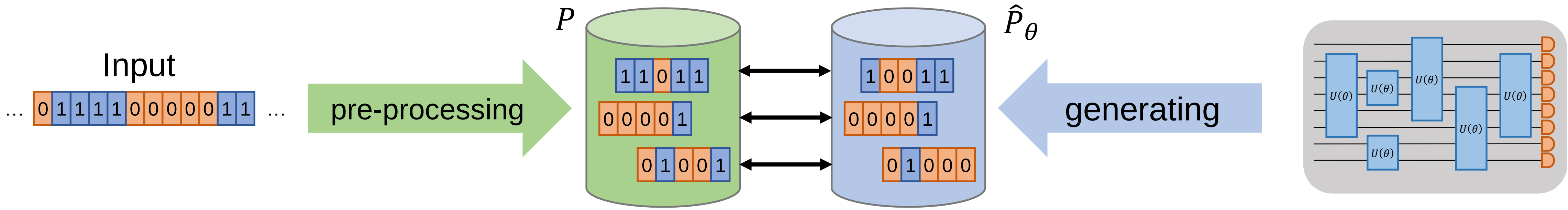
Cost Function

Maximum Mean Discrepancy:
(MMD)



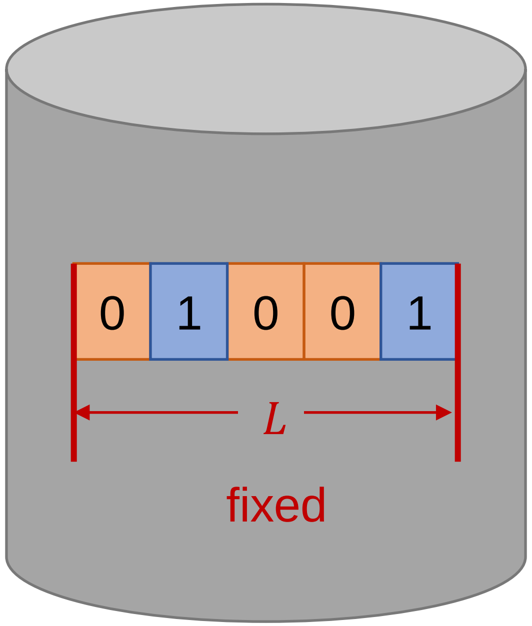


$$\mathrm{MMD}\left[P, \hat{P}\right] = 0 \iff P = \hat{P}$$



Cost Function

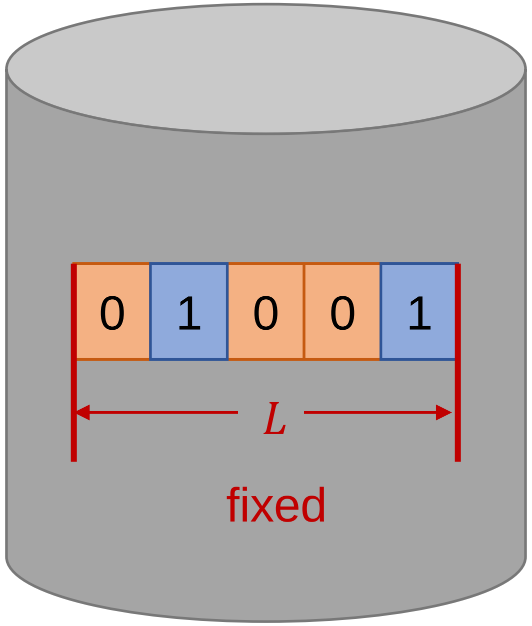
$$C(\boldsymbol{\theta}) = \sum_{\overleftarrow{x}} w_{\overleftarrow{x}} \cdot \mathrm{MMD}^2[\mathrm{P}, \hat{P}_{\boldsymbol{\theta}} | \overleftarrow{x}]$$



Cost Function

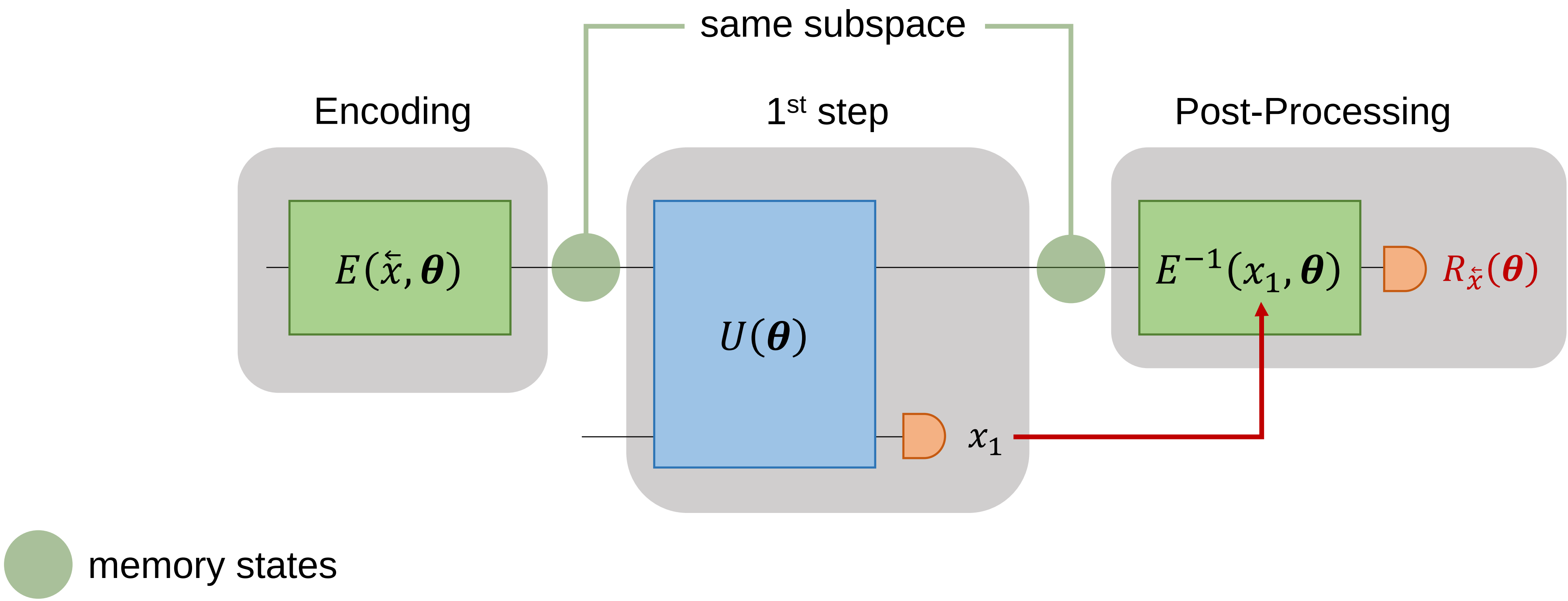
$$C(\boldsymbol{\theta}) = \sum_{\overleftarrow{x}} w_{\overleftarrow{x}} \cdot \mathrm{MMD}^2[\mathrm{P}, \hat{P}_{\boldsymbol{\theta}} | \overleftarrow{x}]$$

$$C(\boldsymbol{\theta}) = \sum_{\overleftarrow{x}} w_{\overleftarrow{x}} \cdot \mathrm{MMD}^2[\mathrm{P}, \hat{P}_{\boldsymbol{\theta}} | \overleftarrow{x}] + R_{\overleftarrow{x}}(\boldsymbol{\theta})$$



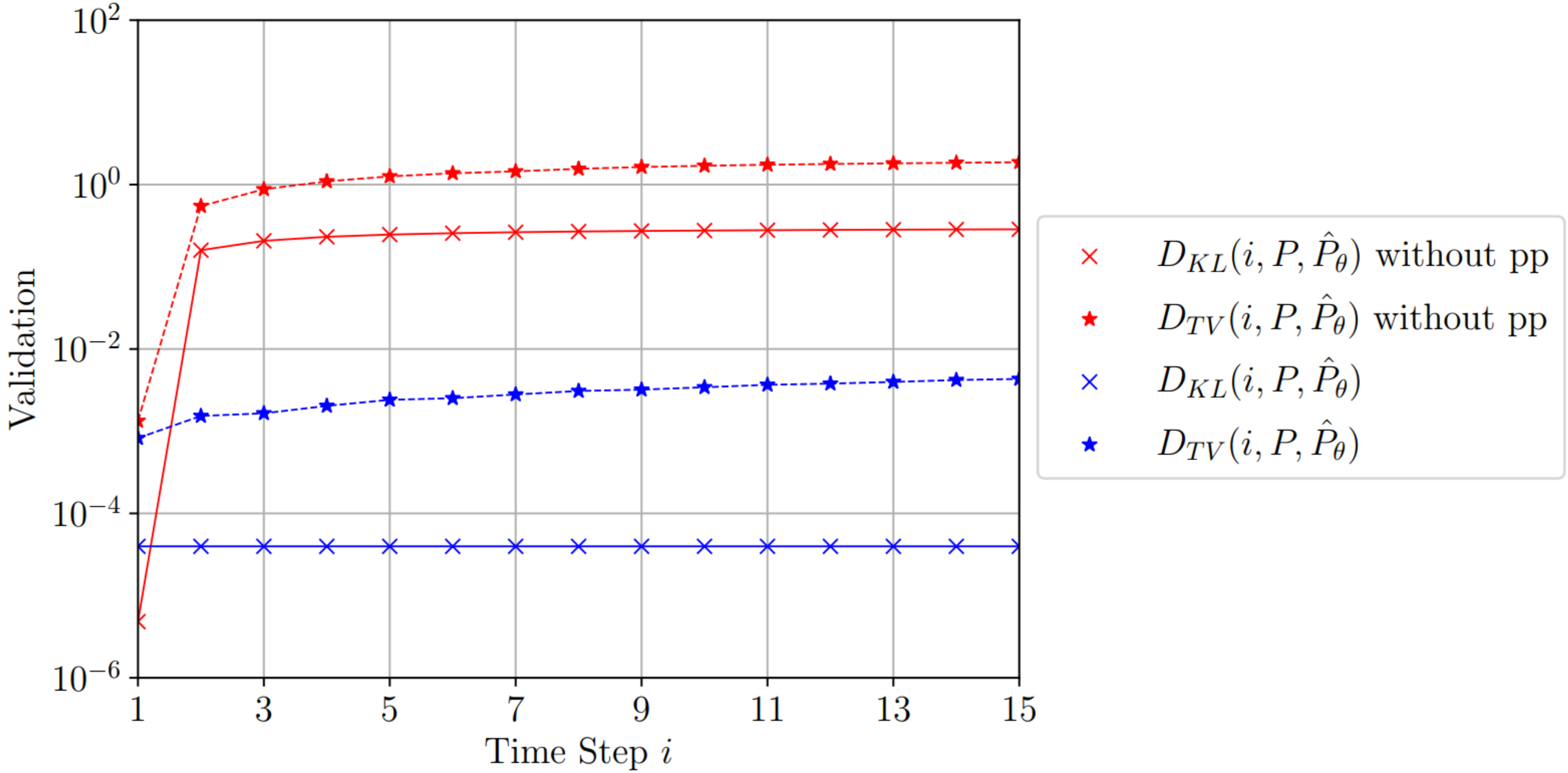
Regularization = penalizes models with a large set of memory states

Cost Function



Results

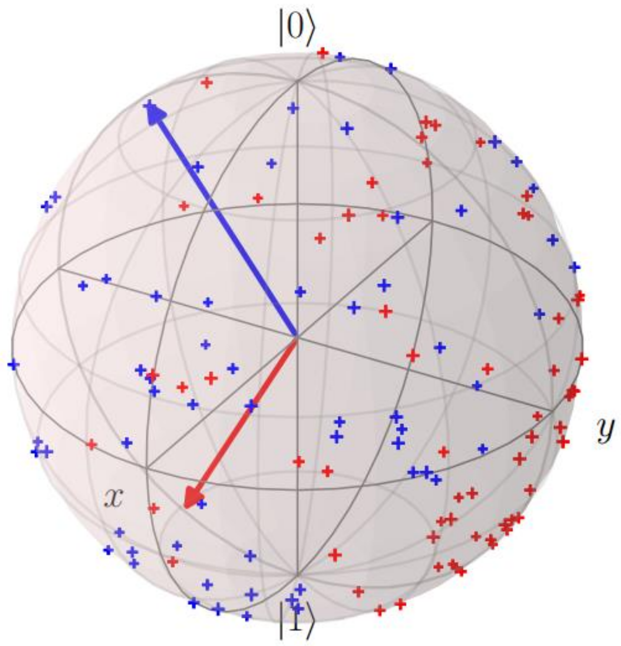
Results



10^2
10^0
10^{-2}
10^{-4}
10^{-6}
Validation
1
3
5
7
9
11
13
15
Time Step i
$D_{KL}(i, P, \hat{P}_\theta)$ without pp
$D_{TV}(i, P, \hat{P}_\theta)$ without pp
$D_{KL}(i, P, \hat{P}_\theta)$
$D_{TV}(i, P, \hat{P}_\theta)$

Results

random



$E(\overleftarrow{x}, \boldsymbol{\theta})$

initial state for $\overleftarrow{x} = 0$

initial state for $\overleftarrow{x} = 1$

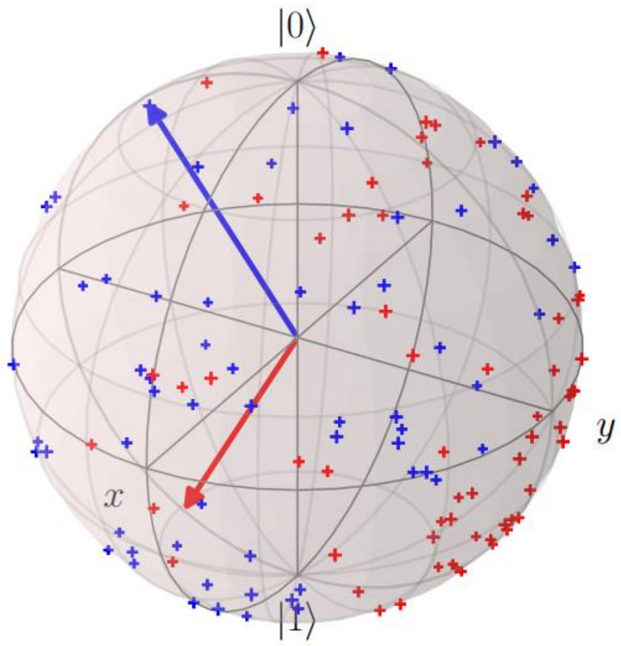
memory states for $x_i = 0$

memory states for $x_i = 1$

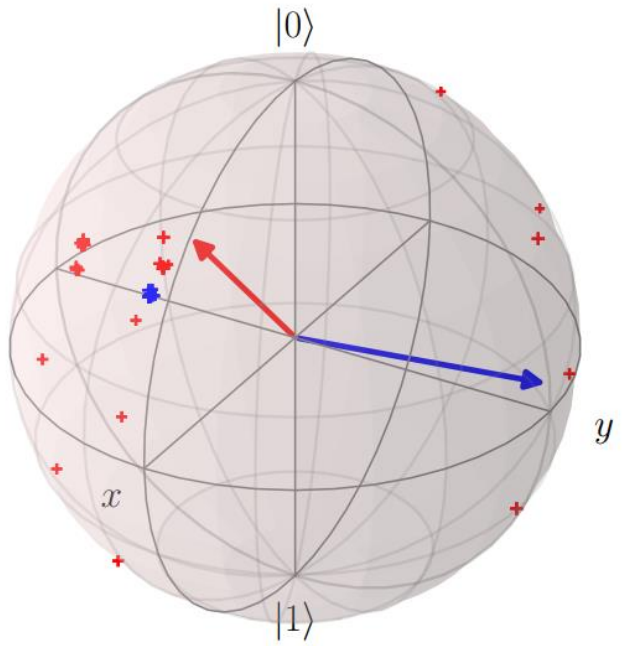
$U(\boldsymbol{\theta})$ | $U(\boldsymbol{\theta})$ | …

Results

random



without pp



$E(\overleftarrow{x}, \boldsymbol{\theta})$

initial state for $\overleftarrow{x} = 0$

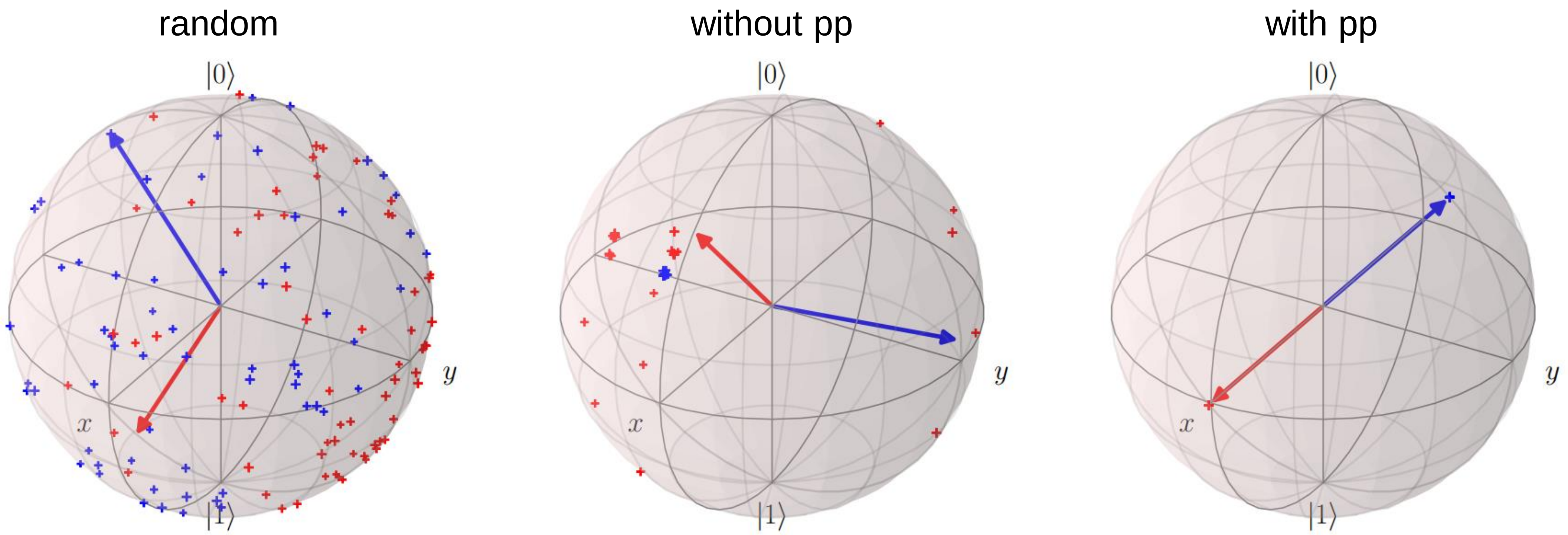
initial state for $\overleftarrow{x} = 1$

memory states for $x_i = 0$

memory states for $x_i = 1$

$U(\boldsymbol{\theta})$ $U(\boldsymbol{\theta})$ …

Results



$E(\overleftarrow{x}, \boldsymbol{\theta})$

initial state for $\overleftarrow{x} = 0$

initial state for $\overleftarrow{x} = 1$

memory states for $x_i = 0$

memory states for $x_i = 1$

$U(\boldsymbol{\theta})$ $U(\boldsymbol{\theta})$ ...

Conclusion & Outlook

- Developed a hybrid quantum learning algorithm for predictive models
- Learning algorithm is memory efficient
- Extended MMD for predictive models → Decrease KL and TV
- Regularization → small set of memory states
- Learned models show constantly good simulation performance

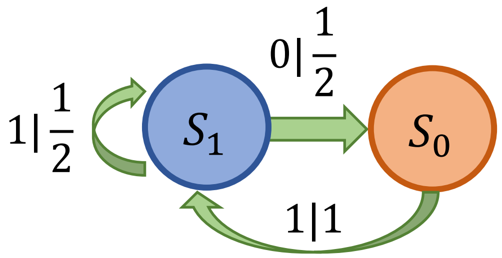
- Apply the algorithm to the period-3 uniform renewal process
- Consider processes with outcomes $\subseteq \mathbb{N}$

Thank you very much!

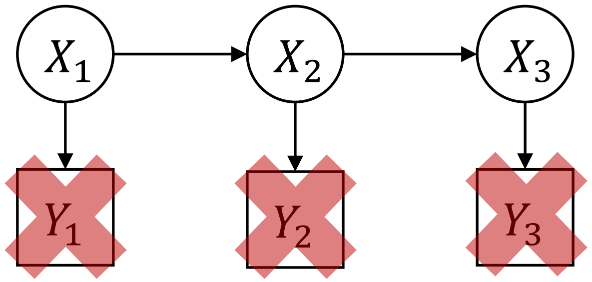
Questions are highly welcome.

ϵ–machine vs. HMM

ϵ-machine



HMM



unifilar

q–simulator

$E(\overleftarrow{x}, \boldsymbol{\theta})$

$$E(\overleftarrow{x})\,|0\rangle = |\sigma_{\overleftarrow{x}}\rangle$$

memory state

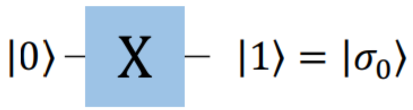
$U(\boldsymbol{\theta})$

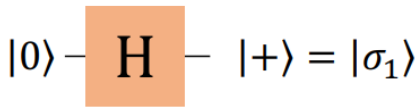
$$T\,|\sigma_{\overleftarrow{x}}\rangle\,|0\rangle = \sum_{x \in A} \sqrt{P(x|\overleftarrow{x})}\,|\sigma_{\overleftarrow{x},x}\rangle\,|x\rangle \xrightarrow{I \otimes M} |\sigma_{\overleftarrow{x},x^*}\rangle\,|x^*\rangle$$

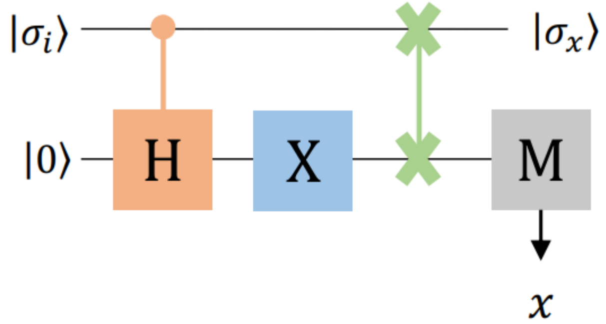
measure

Ansatz

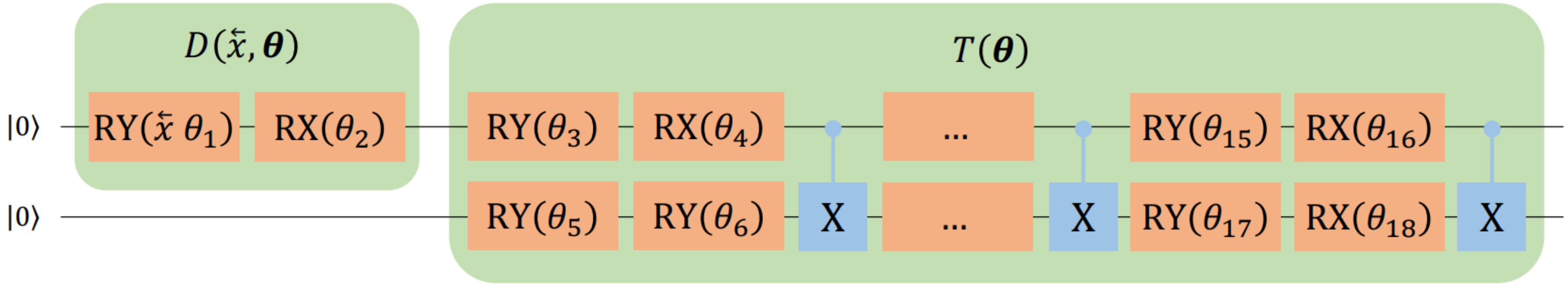
Analytical solution:



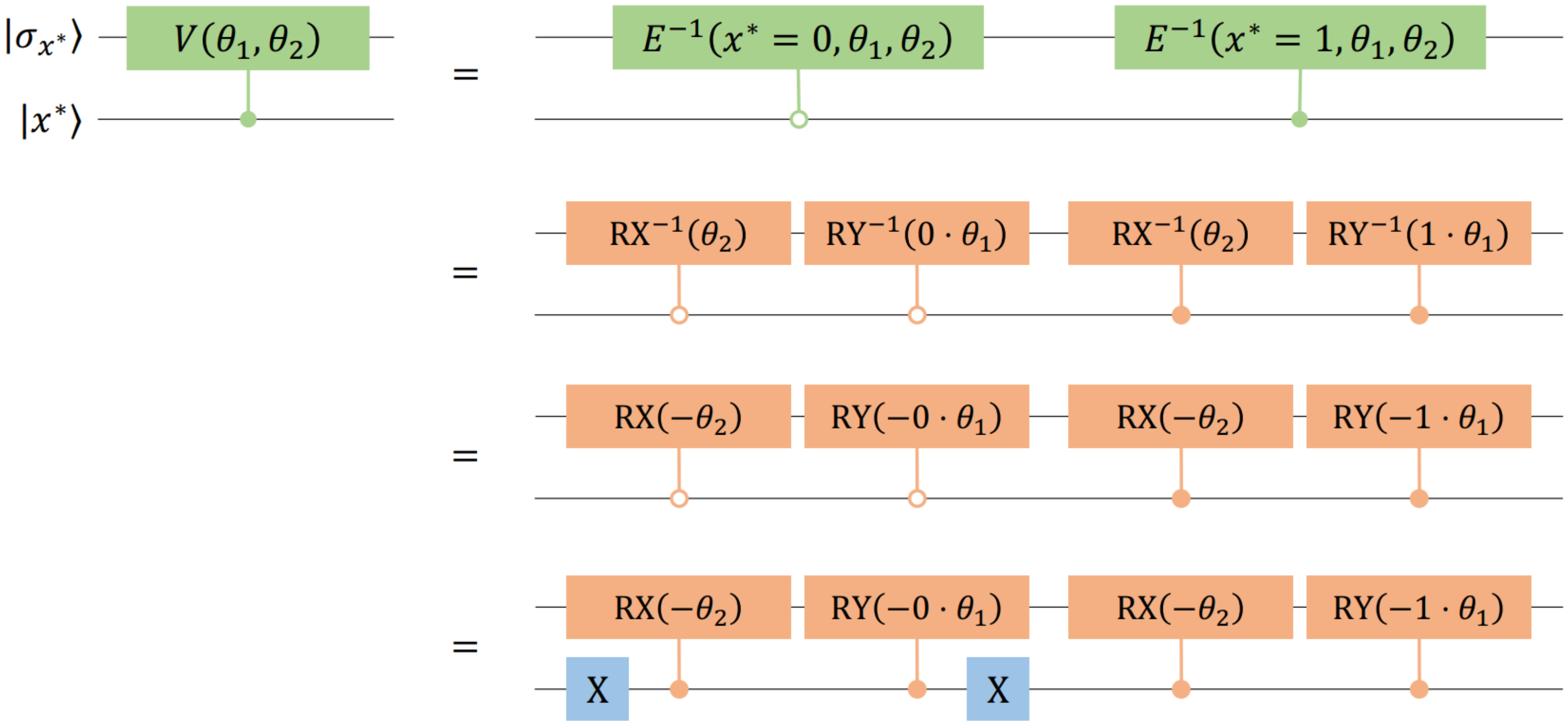




Ansatz:



Post Processing



Validation

Kullback-Leibler divergence: (KL)

$$D_{KL}(P,\hat{P}) = \sum_x P(x)\log_2\frac{P(x)}{\hat{P}(x)}$$

$$D_{KL}(L,P,\hat{P}) = \sum_{x_{1:L}}\frac{1}{L}\sum_{\overleftarrow{x}} P(\overleftarrow{x})\cdot P(x_{1:L}|\overleftarrow{x})\log_2\frac{P(x_{1:L}|\overleftarrow{x})}{\hat{P}(x_{1:L}|\overleftarrow{x})}$$

Total Variation Distance: (TV)

$$D_{TV}(P,\hat{P}) = \frac{1}{2}\sum_x\left|P(x)-\hat{P}(x)\right|$$

$$D_{TV}(L,P,\hat{P}) = \frac{1}{2}\sum_{x_{1:L}}\sum_{\overleftarrow{x}}\left|P(x_{1:L}|\overleftarrow{x})-\hat{P}(x_{1:L}|\overleftarrow{x})\right|$$

Maximum Mean Discrepancy

Kernel

$$MMD^2[F, P, \hat{P}] = \mathbb{E}_{x\sim P, x'\sim P}[k(x, x')] - 2\cdot\mathbb{E}_{x\sim P, y'\sim\hat{P}}[k(x, y)] + \mathbb{E}_{y\sim\hat{P}, y'\sim\hat{P}}[k(y, y')]$$

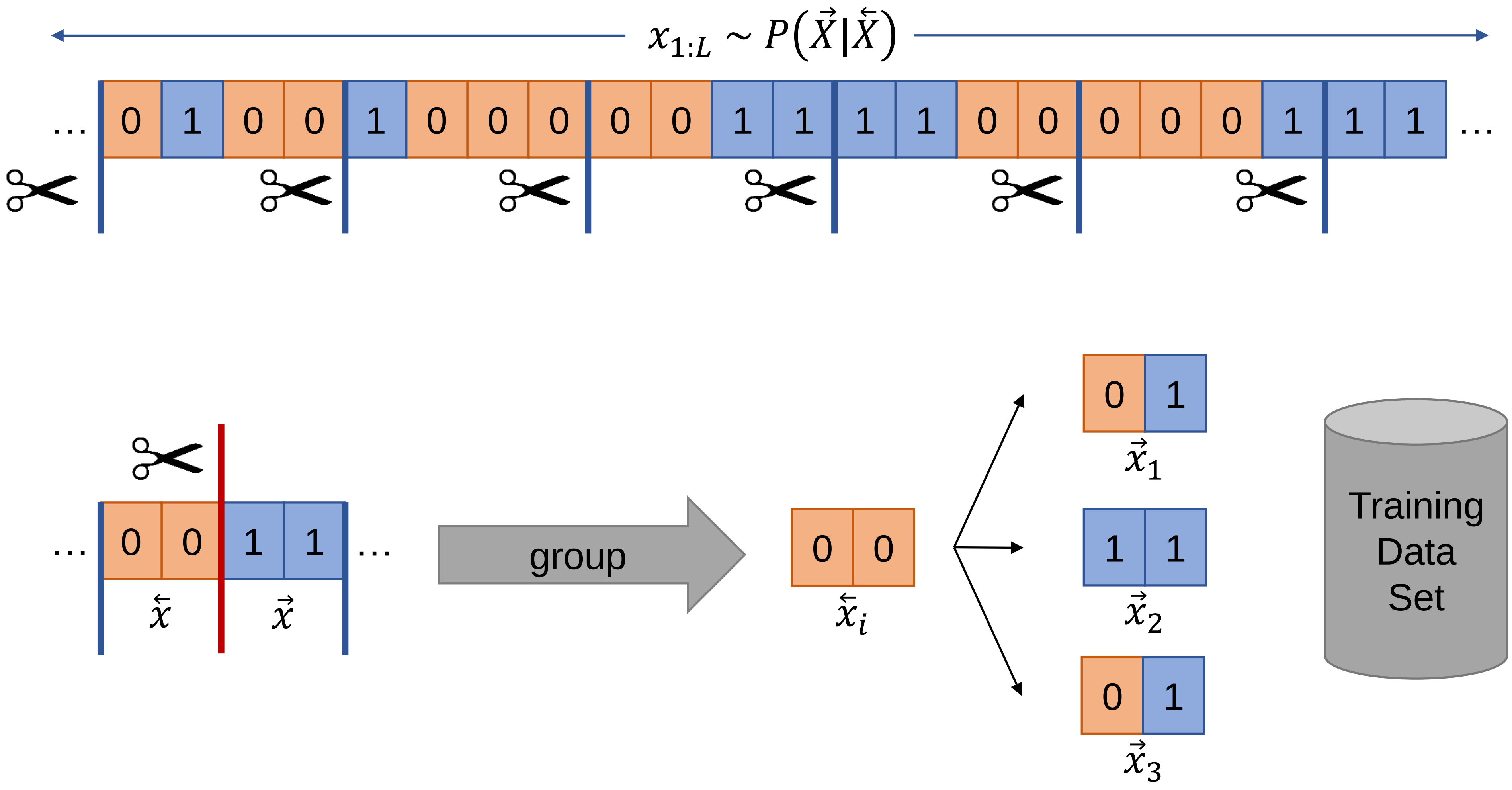
$$\frac{\partial MMD^2[P, \hat{P}_{\boldsymbol{\theta}}]}{\partial\theta_i} = \sum_{j=1}^{m} \alpha'_{i,j}(\theta_i)\left[\underset{\substack{x\sim\hat{P}_{\boldsymbol{\theta}^+_{i,j}} \\ y\sim\hat{P}_{\boldsymbol{\theta}}}}{\mathbb{E}}[k(x, y)] - \underset{\substack{x\sim\hat{P}_{\boldsymbol{\theta}^-_{i,j}} \\ y\sim\hat{P}_{\boldsymbol{\theta}}}}{\mathbb{E}}[k(x, y)] - \underset{\substack{x\sim\hat{P}_{\boldsymbol{\theta}^+_{i,j}} \\ y\sim P}}{\mathbb{E}}[k(x, y)] + \underset{\substack{x\sim\hat{P}_{\boldsymbol{\theta}^-_{i,j}} \\ y\sim P}}{\mathbb{E}}[k(x, y)]\right]$$

Matrix depending on the ansatz

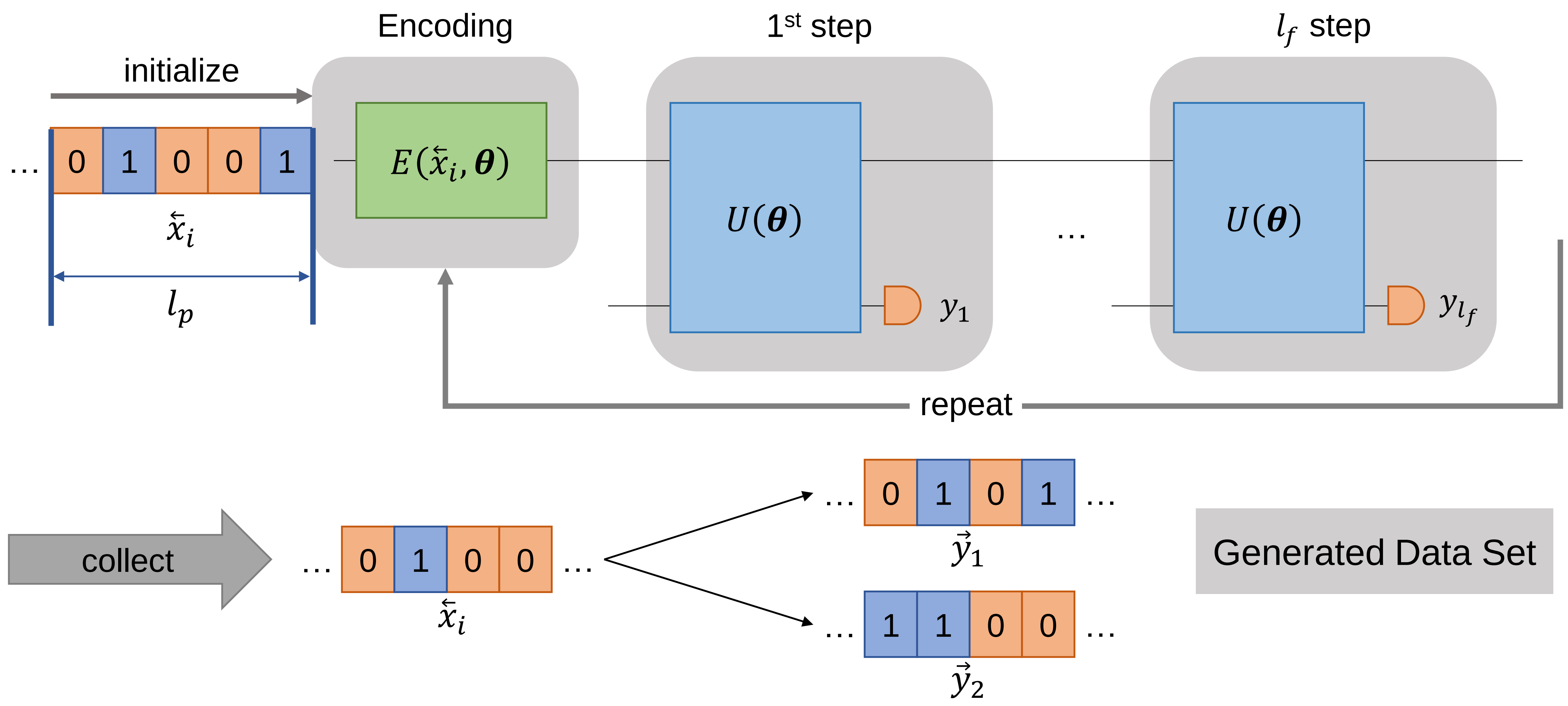
Cost Function

Input:

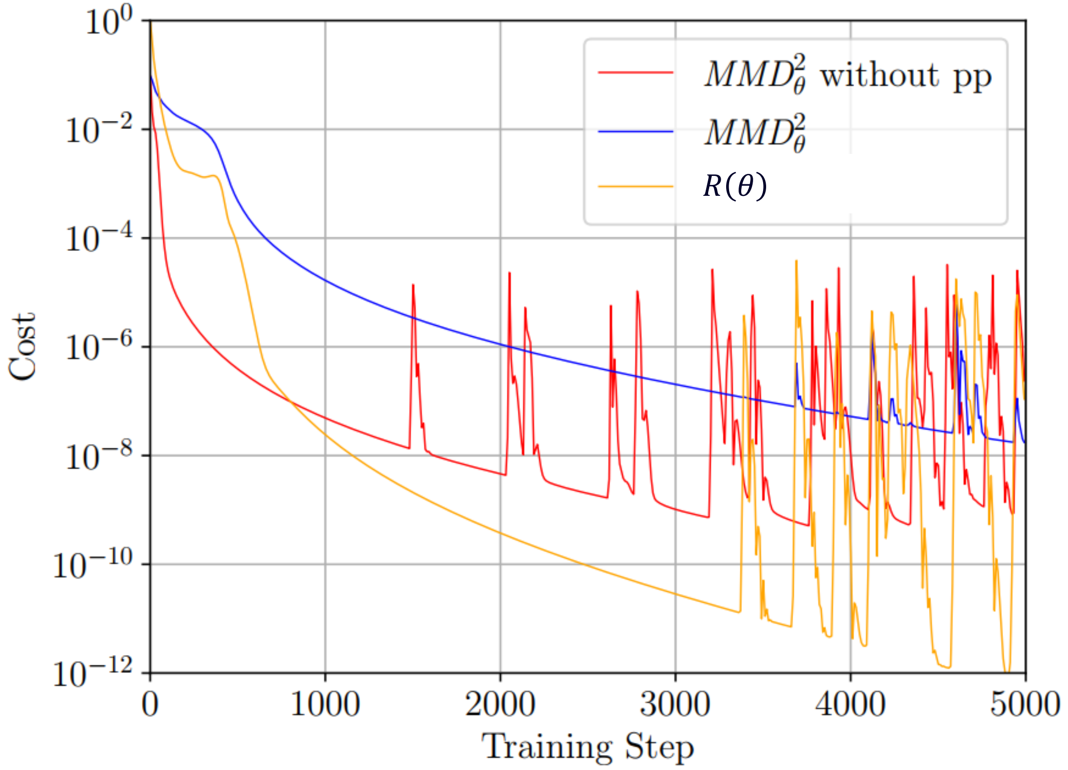
Pre-Processing:



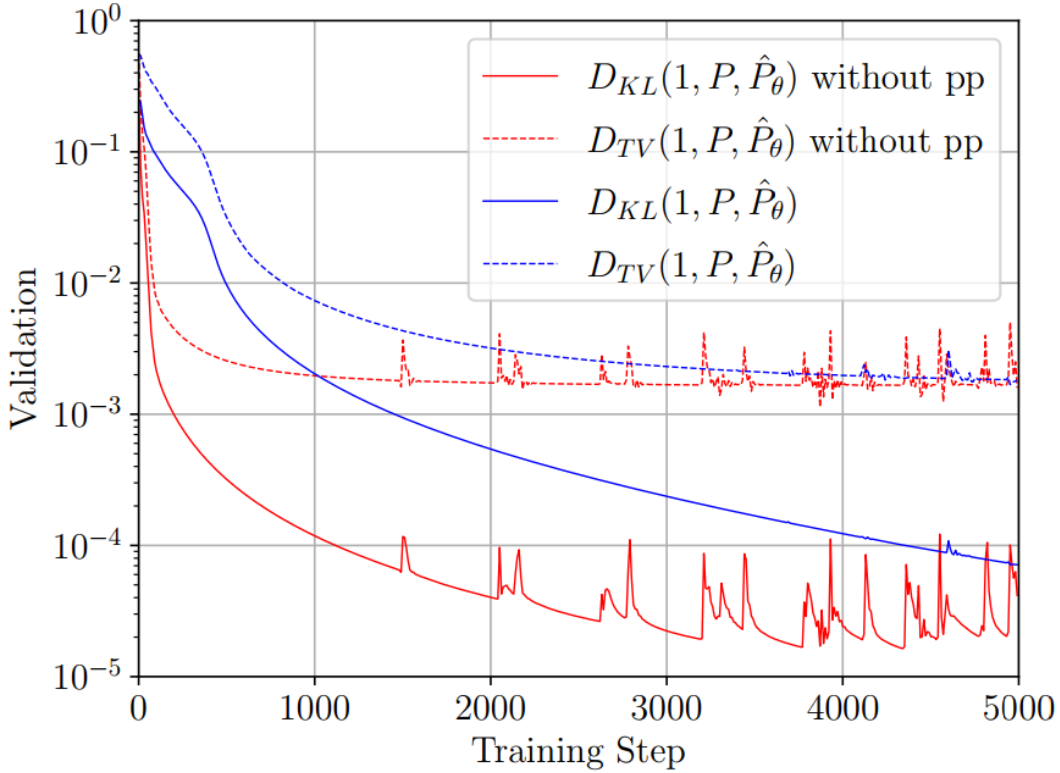
Cost Function



Training

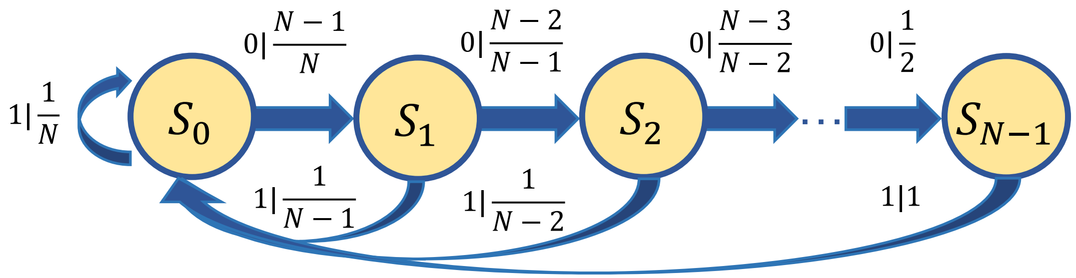


10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
Cost
0
1000
2000
3000
4000
5000
Training Step
MMD_θ^2 without pp
MMD_θ^2
$R(\theta)$



10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Validation
0
1000
2000
3000
4000
5000
Training Step
$D_{KL}(1, P, \hat{P}_\theta)$ without pp
$D_{TV}(1, P, \hat{P}_\theta)$ without pp
$D_{KL}(1, P, \hat{P}_\theta)$
$D_{TV}(1, P, \hat{P}_\theta)$

Period-N Uniform Renewal Process

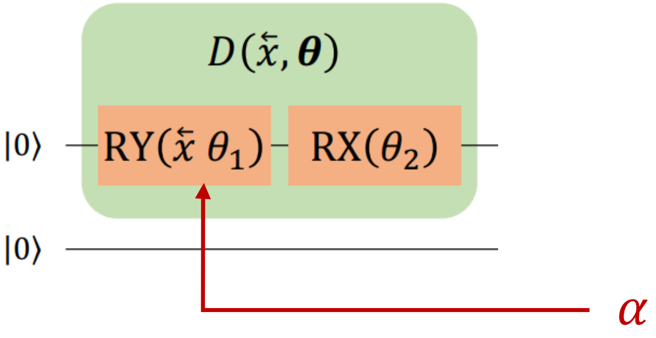


ϵ-machine

Gradients

$$f(\boldsymbol{\theta}) = \langle 0 | U(\boldsymbol{\theta})^{\dagger} \hat{O} U(\boldsymbol{\theta}) | 0 \rangle$$

$$\frac{\partial f(\boldsymbol{\theta})}{\partial \mu} = \frac{1}{2} \sum_{j=1}^{m} \alpha'_j(\mu) \left[f_j\left(\alpha_j(\mu), +\frac{\pi}{2}\right) - f_j\left(\alpha_j(\mu), -\frac{\pi}{2}\right) \right]$$



Thank you very much!

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