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Cluster of Excellence in Data-integrated Simulation Science

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Low-rank approximations of unitary simulators for stochastic processes

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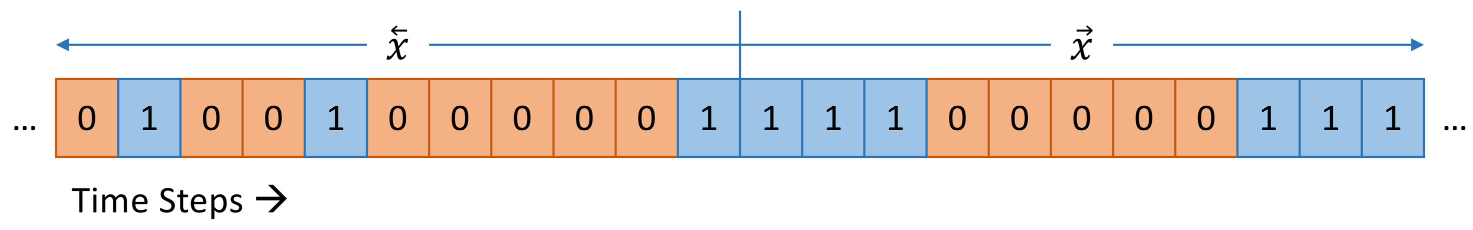
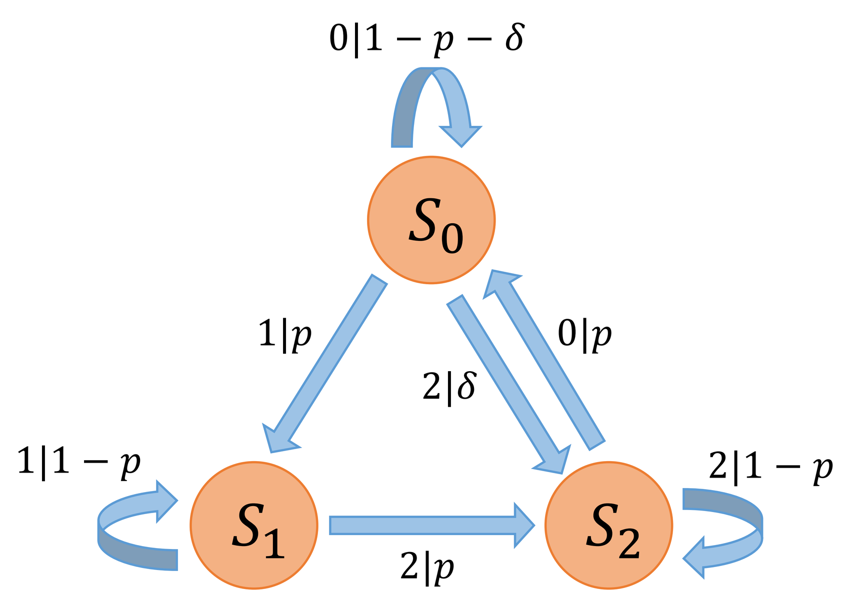
Stochastic Processes

We consider bi-infinite stationary discrete-time stochastic processes with
- a sequence of random variables $X_t \in \mathbb{N}$ with $t \in \mathbb{Z}$
- the *past* defined as $\overleftarrow{X} := \dots, X_{-2}, X_{-1}$
- the *future* defined as $\overrightarrow{X} := X_0, X_1, \dots$
- a governing joint probability distribution $P(\overleftarrow{X}, \overrightarrow{X})$
- a conditional distribution $P(\overrightarrow{X} | \overleftarrow{x})$, given a specific past instance $\overleftarrow{x}$



Example Process



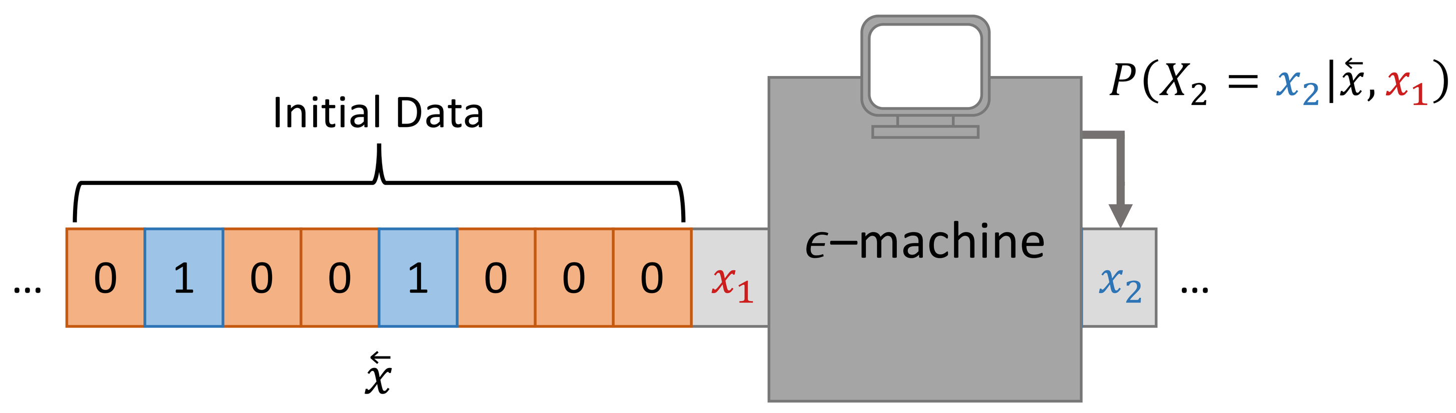
Graphical representation of the *quasi cycle process* with memory states s_i, emissions, and transition probabilities $x|P(x)$.

Classical Models

The provably optimal classical models are ϵ-machines, which are based on the equivalence relation

$$\overleftarrow{x} \sim \overleftarrow{x}' \iff P(\overrightarrow{X}|\overleftarrow{x}) = P(\overrightarrow{X}|\overleftarrow{x}'). \tag{1}$$

For each class, one *memory state* $\mathcal{E}(\overleftarrow{x}) = s_i$ is allocated. The model initializes to a state defined by the input $\overleftarrow{x}$ and outputs a single time step once at a time:

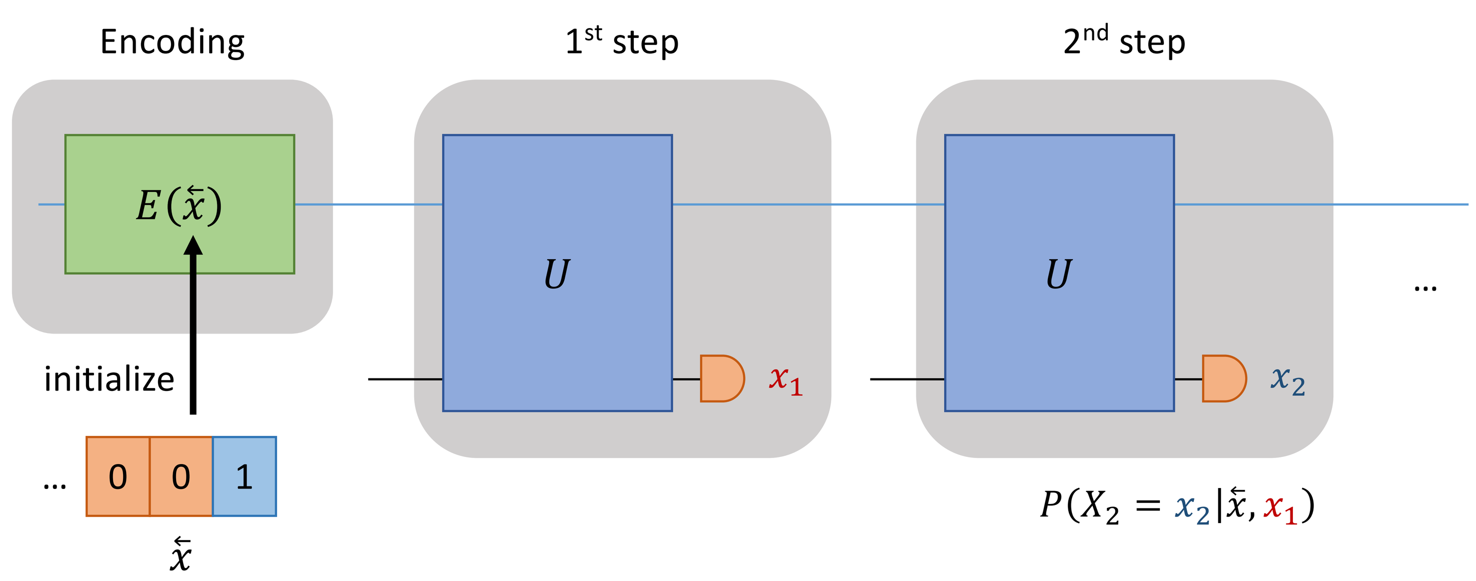


Quantum Models

The quantum analog is called q-simulator and operates onto quantum memory states $|s_i\rangle$ as

$$|1_i\rangle := U\,|s_i\rangle\,|0\rangle = \sum_x \sqrt{P(x|s_i)}\,|s_{\lambda(i,x)}\rangle\,|x\rangle\,, \tag{2}$$

where $\lambda(i, x)$ denotes the index to the next state. A measurement operation onto the second register of $|1_i\rangle$ thus outputs x with probability $P(x|s_i)$:



Low-rank Approximations

We aim for approximate models ($\widehat{P} \approx P$) and start with the following

Theorem [1]: Given a stochastic process with P, λ, and $\{s_i\}_{i=1}^n$. A q-simulator exists iff

$$\langle s_i|s_j\rangle = \langle 1_i|1_j\rangle \qquad \forall\, i, j = 1, 2, \dots, n. \tag{3}$$

→ The main idea of this work is to perform a low-rank approximation of the overlap matrix $C_{i,j} = \langle 1_i|1_j\rangle$ and derive the quantum states $|s_i\rangle$ and unitary simulator U from it.

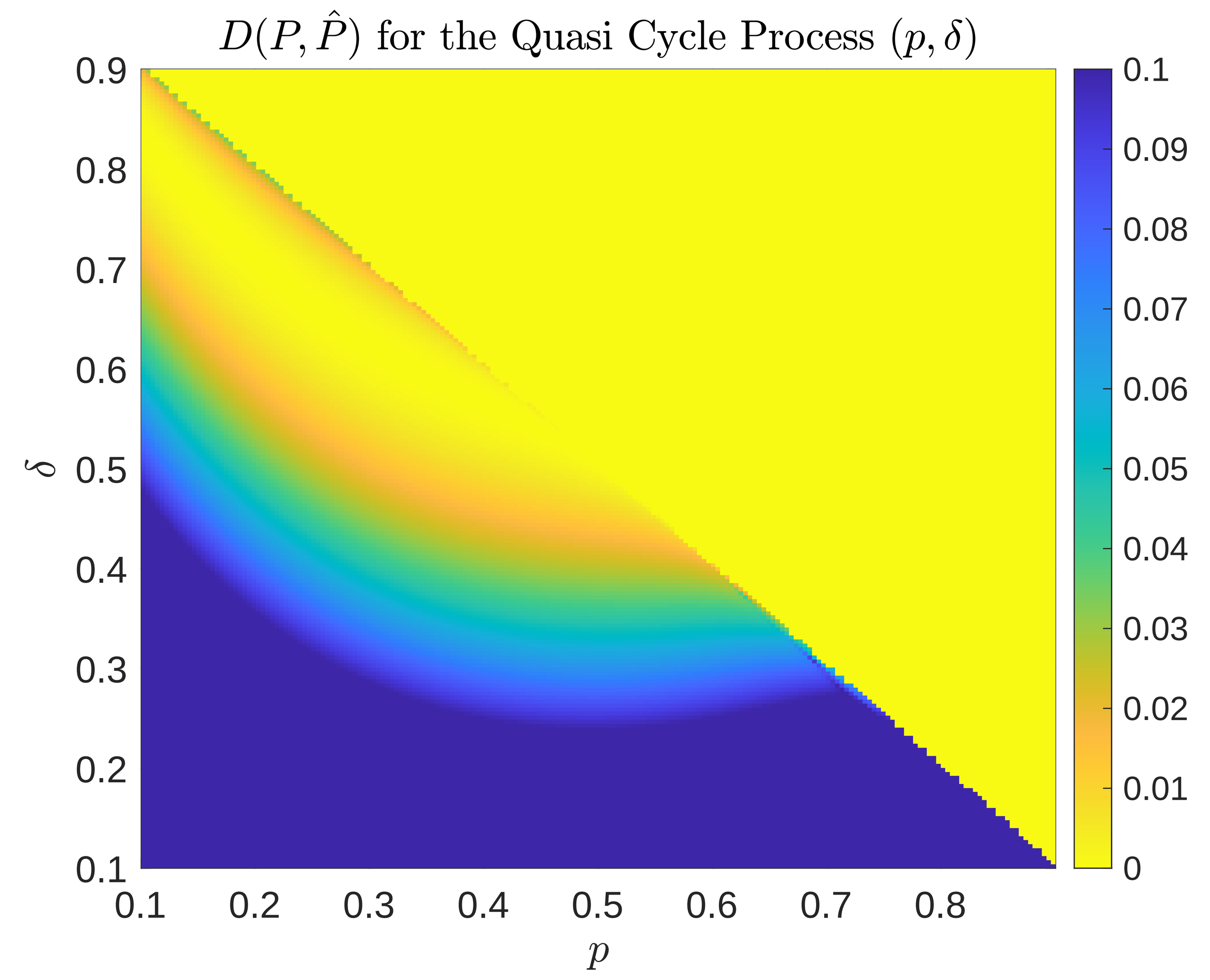
Sketch of the algorithm

1. Construct the overlap matrix $C \leftarrow P, \lambda, \{s_i\}_{i=1}^n$
2. Perform a SVD of $C = V\Sigma W^\dagger = V\Sigma V^\dagger = V\sqrt{\Sigma}\sqrt{\Sigma}V^\dagger$
3. Shrink to a low-rank approximation $C \to C^{(d)} = V\sqrt{\Sigma^{(d)}}\sqrt{\Sigma^{(d)}}V^\dagger$
4. Identify the quantum states $|\widehat{s}_i\rangle$ as columns of $\widehat{S} = \sqrt{\Sigma^{(d)}}V^\dagger$
5. Construct the approximate one-step matrix $\widehat{F}$ with columns $\widehat{F}_i = |\widehat{1}_i\rangle$
6. Approximate the unitary simulator as

$$\underset{\widehat{U}}{\arg\min}\ ||\widehat{U}\widehat{S} \odot |0\rangle - \widehat{F}||_F^2 \qquad \text{s.t.} \qquad \widehat{U}^\dagger\widehat{U} = I \tag{4}$$

Interpretation: The approximate states $|\widehat{s}_i\rangle$ are the quantum states to a slightly different stochastic process $\widehat{P}$ simulated by $\widehat{U}$ following (2).

Results



→ Via comparison with the best classical models [2], these approximate quantum models are superior with respect to the KL divergence

$$D(P, \widehat{P}) = \sum_{\overleftarrow{x}, \overrightarrow{x}} P(\overleftarrow{x})P(\overrightarrow{x}|\overleftarrow{x}) \log_2 \frac{P(\overrightarrow{x}|\overleftarrow{x})}{\widehat{P}(\overrightarrow{x}|\overleftarrow{x})}. \tag{5}$$

Future Directions

- Derive upper bounds onto the KL divergence
- Include complex phases for the overlap matrix C
- Derive QML ansätze to learn approximations based only on data

References

[1] Felix C. Binder, Jayne Thompson, and Mile Gu.
Practical unitary simulator for non-markovian complex processes.
Phys. Rev. Lett., 120:240502, Jun 2018.

[2] Chengran Yang, Andrew J. P. Garner, Feiyang Liu, Nora Tischler, Jayne Thompson, Man-Hong Yung, Mile Gu, and Oscar Dahlsten.
Provably superior accuracy in quantum stochastic modeling.
Phys. Rev. A, 108:022411, Aug 2023.

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