Quantum Rat Vol.3: Learning Dynamics from Measurements

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Motivation

Quantum-like (Q-like) modelling have been applied in decision theory, psychology, and information processing to capture non-classical phenomena such as contextuality and interference [1,4]. Despite their success, the ability to use empirical observations to systematically estimate the Hamiltonian governing system dynamics is often missing. This capability is essential for Q-like modeling to advance beyond conceptual demonstrations toward operational relevance.

The proposed contribution addresses Hamiltonian estimation in a macroscopic setup: the "rat-in-the-box" toy model [2]. The model describes a discrete spatial system in which the rat's movement is driven by a Hamiltonian, which determines the probability distribution that drives the rat. An external observer has access to the realized rat's positions over time and reconstructs the unknown operator from that partial information. Separating objective dynamics (the rat) and the observer's subjective inference makes the proposed interpretable setup a tractable testbed for studying learning strategies.

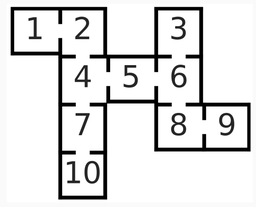


Figure 1: Maze

Quantum–driven Rat in the maze

Maze – a closed non-transparent box with 10 rooms (Fig. 1), some rooms are connected.

Rat moves inside the maze and can occupy one room $x \in \{1, 2, 3, \ldots, 10\}$ at each time, starting at room 1.

- Rat's state is given by $|\psi_{\text{rat}}(t)\rangle \in \mathcal{H}^{10}$ as $|\psi_{\text{rat}}(t)\rangle = \sum_{j=1}^{10} c_j(t)\,|x_j\rangle\,, \quad c_j(t) \in \mathbf{C},\ \sum_{j=1}^{10} |c_j(t)|^2 = 1$, which defines probability distribution $P_{\text{rat}}(t)$ over Rat's positions in maze via Born's rule.
- Rat moves among the rooms according to Hamiltonian $\hat{\text{H}}_{\text{true}}$ as follows:
  - movement: at discrete time t_k Rat samples $x_k \sim P_{\text{rat}}(t_k)$, physically moves to room x_k and Rat's state collapses to $|x_k\rangle$.
  - between movements: Rat's state $|\psi_{\text{rat}}(t)\rangle \in \mathcal{H}^{10}$ evolves unitarily via $\hat{\text{H}}_{\text{true}}$:

$$|\psi_{\text{rat}}(t)\rangle = e^{-i(t-t_k)\hat{\text{H}}_{\text{true}}}\,|\psi_{\text{rat}}(t_k)\rangle\,, \quad t \in (t_k, t_{k+1})\,, \tag{1}$$

    where Hamiltonian $\hat{\text{H}}_{\text{true}}$ is real-valued Hermitian 10-by-10 matrix reflecting maze's structure and Rat's dynamics.
  - after movement: next evolution starts from collapsed state $|\psi_{\text{rat}}(t_{k+1})\rangle \to |x_{k+1}\rangle$

Fig. 2 describes the overall setup. Note that Rat's mind, Rat's neural activity and Rat's effector are distinguished.

Observer

Observer's prior knowledge: structure of the maze (Fig. 1), Rat's initial position ($|\psi_{\text{rat}}(0)\rangle$)

Observer's data: (x_k, t_k) – time sequence of Rat's positions

Observer's task: Make the best estimate of $\hat{\text{H}}_{\text{true}}$ from prior knowledge and data.

Challenge for the Observer:

- **Randomness:** probabilistic sampling and state collapse
- **Ambiguity:** different Hamiltonians can "produce" identical data
- **Small Data:** assumption on invariant $\hat{\text{H}}_{\text{true}}$ in real-life example leads to low amount of data

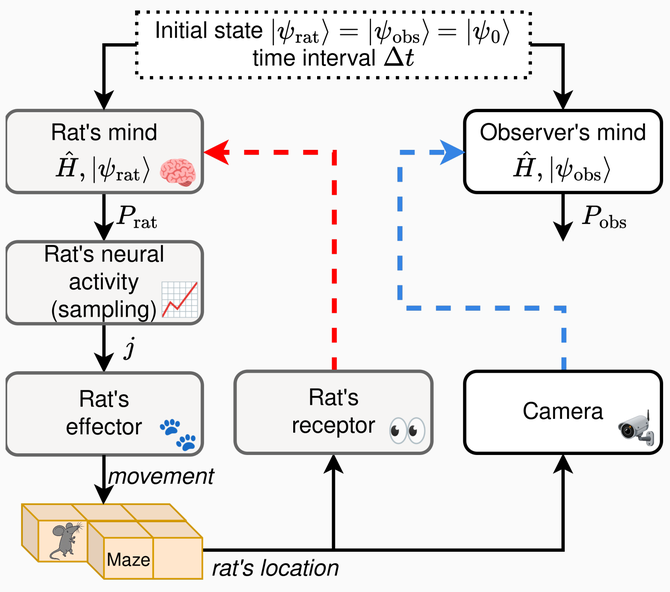


Figure 2: The setup

Estimator III: Bayes–Wishart Estimator

Fully Bayesian treatment where $\hat{\text{H}}$ is modeled as a matrix-variate Wishart distribution $\mathcal{W}_N(\nu, \mathbb{S})$.

Initialization: Prior belief: $\hat{\text{H}} \sim \mathcal{W}_N(\nu_0, \mathbb{S}_0)$ with $\mathbb{E}[\hat{\text{H}}] = \mathbb{S}_0$ and $\nu_0 = N + 1$ reflects minimal initial knowledge.

Update loop (per observation $x_{k-1} \to x_k$ at time t_k):

1. **Monte-Carlo Sampling:** Draw M candidate Hamiltonians $\{\hat{\text{H}}_m\}_{m=1}^M$ from Wishart prior $\mathcal{W}_N(\nu, \mathbb{S})$ via Cholesky decomposition ($\hat{\text{H}} = \mathbb{C}^\top\mathbb{C}$).
2. **Likelihood weights** are transition probabilities for each sample: $w_m^2 = |\,\langle x_k|\, e^{-i\hat{\text{H}}_m t_k}\,|x_{k-1}\rangle\,|^2$
3. **Posterior Projection:** Fit new Wishart $\mathcal{W}_N(\nu + 1, \mathbb{S}_{\text{new}})$ to weighted sample by preserving:

$$\mathbb{S}_{\text{new}} \approx \frac{\sum_m w_m^2 \mathbb{C}_m^\top \mathbb{C}_m}{\sum_m w_m^2} \tag{2}$$

4. **Geometric Pooling with Forgetting:** Merge $\mathbb{S}_{\text{new}}$ and $\mathbb{S}$ using adaptive forgetting factor $\phi \in (0, 1)$:

$$(\nu + \phi)\mathbb{P} = \phi(\nu + 1)\mathbb{S}_{\text{new}} + (1 - \phi)\nu\mathbb{S}, \quad \mathbb{S}_{\text{final}} = \mathbb{P}^{-1} \tag{3}$$

5. **Maze structure enforcement:** Respect maze topology (impossible transitions are set to 0).

👍 maintains full covariance structure of parameter uncertainty, enabling risk-aware decision-making under small data.

Estimator I: MLE Approach

Regularized Maximum Likelihood Estimation incorporates structural priors via an L_2 penalty to prevent overfitting. We optimize over the parameter vector $\boldsymbol{\theta}$ defining the Hamiltonian $\hat{\text{H}}_{\text{est}}(\boldsymbol{\theta})$:

$$\boldsymbol{\theta}_{\text{est}} = \arg\min_{\boldsymbol{\theta}} \left(-\log \mathcal{L}(\boldsymbol{\theta}) + \lambda\|\boldsymbol{\theta}\|^2\right)\,,\ \lambda > 0,$$

where the log-likelihood aggregates transition probabilities across N measurements:

$$\log \mathcal{L}(\boldsymbol{\theta}) = \sum_{k=1}^{N} \log \left|\langle x_{k+1}|\, e^{-iH(\boldsymbol{\theta})\tau_k}\,|x_k\rangle\right|^2. \tag{4}$$

Constrained parameterization enforces sparsity matching the maze structure.

Estimator II: Quantum Hamiltonian Learning

Hybrid quantum-classical optimization that uses parameterized circuits to simulate $\hat{\text{H}}$ evolution natively. Two estimators: ideal simulation and noisy hardware execution.

Hamiltonian Encoding: $\hat{\text{H}}$ is mapped to single-excitation subspace via Pauli operators $\hat{\text{X}}, \hat{\text{Y}}, \hat{\text{Z}}$:

$$\hat{\text{H}}_{\text{est}} = \sum_i \alpha_i \hat{\text{Z}}_i + \sum_{i<j} \beta_{ij}(\hat{\text{X}}_i\hat{\text{X}}_j + \hat{\text{Y}}_i\hat{\text{Y}}_j), \tag{5}$$

where α_i reflects room "attractivity" while β_{ij} transition strengths.

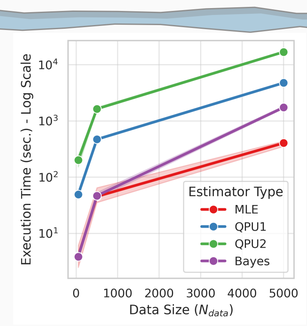
Algorithm:

1. Build $e^{-i\hat{\text{H}}_{\text{est}}t}$ via Trotter-Suzuki decomposition.
2. Run on simulator (QPU1) or transpile for real QPU (QPU2) with error mitigation.
3. Minimize negative log-likelihood using derivative-free optimizer w.r.t. observed trajectory.

Criterion of quality

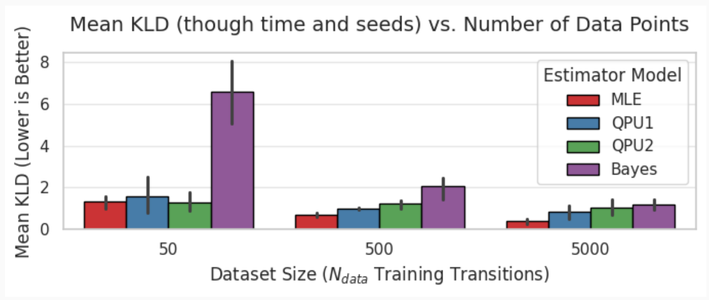
Observer's estimate $\hat{\text{H}}_{\text{est}}$ of $\hat{\text{H}}_{\text{true}}$ is good if for several subsequent validation epochs the respective distributions are close in KLD sense:

$$\text{KLD}\left(P_{\text{rat}}(t)\,||\,P_{\text{est}}(t)\right) \approx 0 \tag{6}$$



🤔 QPU2 performance validated on IBM fake backend (CPU-simulated). Preliminary real-QPU runs confirm superior scalability and faster execution times compared to classical simulation.

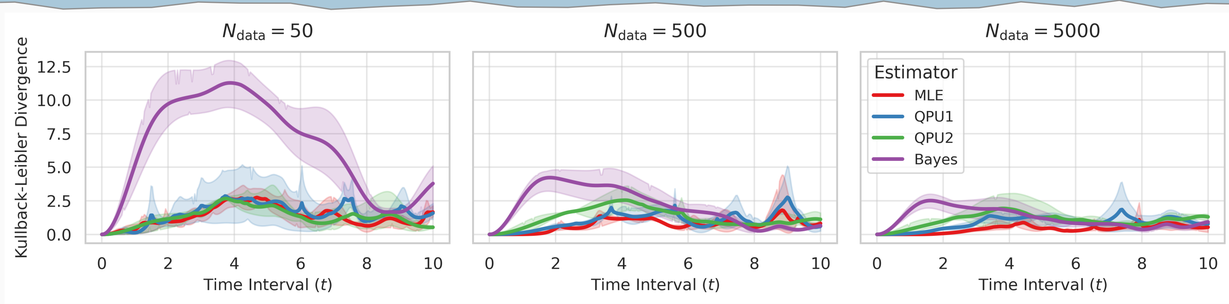
Simulation results



🤔 How to evaluate/compare the results?

🤔 Should standard Markov chain be considered?

All estimators assume collapse. 🤔 how to generalize this?



🤔 Why is Bayes estimator so biased for small data? 🤔 What is a realistic N for real, individual-centric Q-like task?

Concluding Remarks

- 3 Hamiltonian estimators built and tested on Q-like problem
- Reliable H_{est} requires big data – often impossible in Q-like problems.
- Preliminary results indicate the need to exploit all knowledge (domain knowledge, physical models, ...) for learning Q-like systems.

References

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