

Lindlad, Noise and possible links with PMMs

Collaboration on Noise, Open quantum systems and more

November 2

1 Introduction

This note provides an extremely abridged, and perhaps overly practical, introduction to open quantum systems. The goal is to provide the basis for understanding and implementing an open quantum system using the Lindblad master equation. And then hopefully link this with PMMs.

2 Open?

In quantum mechanics, a system is considered *closed* if it is isolated from its environment. In contrast, an *open quantum system* interacts with its environment, which can cause the system to lose coherence and entanglement.

All this boils down to whether or not energy is conserved. In a closed system, energy is conserved, while in an open system, energy is not conserved.

3 Density Matrices

As opposed to the wavefunction (a so-called pure state) in closed (Hermitian) quantum mechanics, the density matrix uniquely describes the state of a quantum system in an open system, as well as in closed systems.

With pure states, the state of a quantum system is deterministic and leads to probabilities of outcomes of measurements. In contrast, what if the state itself is uncertain and therefore probabilistic? This is what density matrices describe.¹

The important properties are summarized here:

- The density matrix of a pure state $|\psi\rangle$ is $\rho = |\psi\rangle\langle\psi|$.
- ρ is Hermitian, positive semi-definite (all eigenvalues non-negative), and has unit trace:

$$\rho = \rho^\dagger, \quad \lambda(\rho) \geq 0, \quad \text{Tr}(\rho) = 1.$$

- Given a probabilistic mixture of states with probabilities $\{p_i\}$ and states $\{|\psi_i\rangle\}$,

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|.$$

¹A natural question might be: “What about probabilistic mixtures of density matrices?” Luckily, such systems are also just described by density matrices.

- For a $d \times d$ density matrix ρ , there exists an orthonormal basis $\{|b_i\rangle\}$ such that

$$\rho = \sum_i \lambda_i |b_i\rangle \langle b_i|,$$

where λ_i are probabilities.

- The expectation value of an observable X is

$$\langle X \rangle = \text{Tr}(\rho X) = \sum_i \lambda_i \langle b_i | X | b_i \rangle.$$

- The time evolution in a closed system with Hamiltonian H is

$$\rho(t) = e^{-iHt} \rho(0) e^{iHt}.$$

3.1 One Qubit Example

The codes for these various examples are included as a separate Python code.. Consider a single qubit system that has a 50% chance of being in $|0\rangle$, a 25% chance of being in $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and a 25% chance of being in $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Then

$$\rho = \frac{1}{2} |0\rangle \langle 0| + \frac{1}{4} |+\rangle \langle +| + \frac{1}{4} |-\rangle \langle -| = \begin{bmatrix} 3/4 & 0 \\ 0 & 1/4 \end{bmatrix}.$$

3.2 Two Qubit Example

Consider a system of two qubits that has a 90% chance of being in the Bell state

$$|B_+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

The remaining 10% is distributed among $|01\rangle$, $|10\rangle$, and $|B_-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$ in the ratio 3:2:1. Then

$$\rho = \frac{9}{10} |B_+\rangle \langle B_+| + \frac{1}{20} |01\rangle \langle 01| + \frac{1}{30} |10\rangle \langle 10| + \frac{1}{60} |B_-\rangle \langle B_-|.$$

4 Subsystems and Partial Traces

An open quantum system is a subsystem of a closed system composed of system + environment. To describe only the system, we trace out the environment:

$$\rho_A = \text{Tr}_B(\rho).$$

For a pure state $|\psi\rangle = |a\rangle \otimes |b\rangle$, the reduced density matrix is

$$\rho_A = \sum_j (I_A \otimes \langle j|) \rho (I_A \otimes |j\rangle).$$

4.1 Two Qubit Example

From the two-qubit example,

$$\rho_1 = \text{Tr}_2(\rho) = \begin{bmatrix} 61/120 & 0 \\ 0 & 59/120 \end{bmatrix}, \quad \rho_2 = \text{Tr}_1(\rho) = \begin{bmatrix} 59/120 & 0 \\ 0 & 61/120 \end{bmatrix}.$$

5 von Neumann Equation

For the total density matrix ρ_T of system plus environment with total Hamiltonian H_T ,

$$\frac{d\rho_T}{dt} = -i[H_T, \rho_T].$$

6 Lindblad Master Equation

Writing $H_T = H + H_E + H_I$, where H is the system Hamiltonian, H_E the environment Hamiltonian, and H_I their interaction, tracing out the environment and assuming weak coupling yields:

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k \gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right),$$

where ρ is the reduced density matrix, $\gamma_k \geq 0$ are decay rates, and L_k are jump operators.

The Heisenberg picture form is

$$\frac{dX}{dt} = i[H, X] + \sum_k \gamma_k \left(L_k^\dagger X L_k - \frac{1}{2} \{L_k^\dagger L_k, X\} \right),$$

and the identity operator satisfies $\frac{dI}{dt} = 0$.

6.1 Liouvillian Superoperator

Define the superoperator \mathcal{L} by

$$\mathcal{L}[\rho] = -i[H, \rho] + \sum_k \gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right),$$

so that

$$\frac{d\rho}{dt} = \mathcal{L}[\rho].$$

6.2 Vectorization: The Fock–Liouville Space

Define $|A\rangle\rangle\rangle$ as the column-stacked vectorization of an operator A . The inner product is

$$\langle\langle A | B \rangle\rangle\rangle = \text{Tr}(A^\dagger B),$$

and

$$\frac{d}{dt} |\langle\rho\rangle\rangle = \hat{\mathcal{L}} |\langle\rho\rangle\rangle,$$

with solution

$$\langle\rho(t)\rangle = e^{\hat{\mathcal{L}}t} \langle\rho(0)\rangle.$$

Diagonalizing $\hat{\mathcal{L}}$ gives eigenvalues λ_i and eigenvectors $\langle r_i \rangle$ and $\langle l_i \rangle$, allowing

$$\langle\rho(t)\rangle = \sum_i e^{\lambda_i t} \langle l_i | \rho(0) \rangle \langle r_i \rangle.$$

6.3 Steady State

The steady state $\langle\rho_{ss}\rangle$ satisfies

$$\hat{\mathcal{L}} \langle\rho_{ss}\rangle = 0.$$

6.4 Harmonic Oscillator Coupled to a Bath

For $H = \omega a^\dagger a$ and jump operators $L_1 = \sqrt{\gamma(\tau+1)} a$, $L_2 = \sqrt{\gamma\tau} a^\dagger$, the Lindblad equation reads:

$$\frac{d\rho}{dt} = -i[\omega a^\dagger a, \rho] + \gamma(\tau+1) \left[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\} \right] + \gamma\tau \left[a^\dagger \rho a - \frac{1}{2}\{aa^\dagger, \rho\} \right].$$

7 Possible roadmap for beyond zero noise extrapolation for quantum computing using PMMs

In the Noisy Intermediate Scale Quantum (NISQ) computing era, error mitigation is vital to obtain meaningful results from quantum algorithms running on existing hardware. This project aims to develop a Parametric Matrix Model (PMM) which learns the underlying open quantum system nature of today's noisy quantum computers in order to better understand the sources of error and directly extrapolate to results with zero noise.

Quantum gates are often modeled idealistically as unitary operators acting on a quantum state. However, in practice, quantum gates are subject to noise which can be modeled as a quantum channel. The noise can be characterized by a superoperator acting on the density matrix of the quantum state. There are many equivalent formalisms including the Liouville superoperator and the Kraus operator sum [?].

A simplified mathematical overview is that if a noiseless operation can be represented as a unitary operator U acting on a pure state $|\psi\rangle$,

$$|\psi\rangle \rightarrow U|\psi\rangle,$$

then a noisy operation can be represented as a superoperator S acting on a vectorized density matrix $|\rho\rangle$,

$$|\rho\rangle \rightarrow S|\rho\rangle.$$

Vectorization is a central operation in the Liouville formalism. The vectorization of a matrix A is formed by stacking the columns of A into a single column vector.

Any noiseless quantum circuit can be represented by a product of unitary operators U_1, U_2, \dots, U_n

acting on the initial state $|\psi_0\rangle$,

$$|\psi_0\rangle \rightarrow U_n U_{n-1} \cdots U_1 |\psi_0\rangle.$$

The corresponding noisy circuit can be represented by a product of superoperators S_1, S_2, \dots, S_n acting on the vectorized initial density matrix $|\rho_0\rangle\rangle$,

$$|\rho_0\rangle\rangle \rightarrow S_n S_{n-1} \cdots S_1 |\rho_0\rangle\rangle.$$

Unitary operators have many nice properties such as:

- $U^\dagger U = UU^\dagger = I$ (unitarity),
- $\lambda(U) = \{e^{i\theta} : \theta \in \mathbb{R}\}$ (eigenvalues on the unit circle),
- $\|Ux\|_2 = \|x\|_2$ (norm preservation).

In contrast, superoperators for quantum channels must be *completely positive and trace preserving* (CPTP). For a map $\Phi : L(H) \rightarrow L(H)$, this means:

- For any positive semidefinite operator X , $\Phi(X)$ is also positive semidefinite.
- For any Hilbert space H' , $\Phi \otimes I_{H'}$ is also positive.
- $\text{tr}(\Phi(X)) = \text{tr}(X)$ (trace preserving).

Completely positive maps are always positive, and every CPTP map represents a valid quantum channel. The matrix representation of a superoperator can be reshaped into a positive semidefinite matrix, guaranteeing complete positivity. Other properties, such as trace preservation and Hermiticity preservation, arise from related transformations.

Choosing a formalism and parameterization that respects these properties is crucial for any PMM that aims to learn the underlying noise model of a quantum computer.

The goal of this project is to develop a PMM that can learn (perhaps a low-dimensional representation of) the underlying open quantum system nature of a real quantum circuit on a real quantum computer. Using this, we aim to demonstrate zero-noise extrapolation using the PMM that is more physically constrained and potentially more accurate than current state-of-the-art ZNE techniques.

By learning the underlying noise model of each gate on a physical quantum computer, we can potentially use this information to construct circuits that are more robust to noise.

8 Project Plan

8.1 Implementing Hamiltonians onto a Circuit

Once Qiskit basics are understood, implement a Hamiltonian onto a circuit. Start with the Transverse Field Ising Model:

$$H = B \sum_i X_i + J \sum_i Z_i Z_{i+1},$$

where X and Z are Pauli operators. See Ref. [?] for guidance on encoding many-body Hamiltonians.

8.2 Zero-Noise Extrapolation

Study sources of noise during computation and the presence of different noise channels. A useful reference is Nielsen and Chuang's *Quantum Computation and Quantum Information*. The depolarizing noise channel is typically used in ZNE. Implement ZNE following Ref. [?], or use the `mitiq` Python library (<https://mitiq.readthedocs.io/>).

If time allows, perform a literature search on ZNE techniques enhanced with neural networks (recent results within the last 1–2 years) to include as comparison.

8.3 Exact Simulation of Simple Circuit

Implement an exact unitary simulation of a simple circuit, such as Bell-state generation and measurement. Then extend it to an exact noisy simulation.

8.4 PMM for Noiseless Simple Circuit

Implement a PMM for the noiseless circuit and train it to reproduce observables or states. Explore larger circuits to study potential dimensionality reduction.

8.5 PMM for Noisy Simple Circuit

Develop a PMM for the noisy circuit. Demonstrate that it can learn the underlying noise model and extrapolate to the noiseless case. Explore larger circuits as before.

8.6 Comparison with Traditional ZNE

Compare PMM performance with traditional ZNE methods for the simple circuit. This may involve real quantum hardware or realistic noise simulators.

8.7 Real Hardware

Demonstrate the PMM method on real quantum hardware, comparing it with existing ZNE techniques such as those in `mitiq`. If necessary, use tensor-network approaches (MPS, DMRG, TEBD) to reduce computational complexity.

References

References

- [1] D. Manzano, *A Short Introduction to the Lindblad Master Equation*, arXiv:1906.04478, 2020.
- [2] H. Yuen, *Lecture 2: Mixed States and Density Matrices*, 2022.

- [3] T. Giurgica-Tiron, Y. Hindy, R. LaRose, A. Mari, and W. J. Zeng, “Digital zero noise extrapolation for quantum error mitigation,” in *IEEE International Conference on Quantum Computing and Engineering (QCE)*, pp. 306–316, 2020.
- [4] A. Smith, M. S. Kim, F. Pollmann, and J. Knolle, “Simulating quantum many-body dynamics on a current digital quantum computer,” *npj Quantum Information*, 5(1):106, 2019.
- [5] C. J. Wood, J. D. Biamonte, and D. G. Cory, “Tensor networks and graphical calculus for open quantum systems,” 2015.