Model order reduction methods for Lindblad type equations

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Motivation: fault-tolerant quantum computing

Contrary to classical bits that are either 0 or 1, *quantum* bits (qubits) are unit vectors of the two-dimensional space $\mathbb{C}^2 = \mathrm{Span}\,(|0\rangle, |1\rangle)$. As a classical bit can be encoded into the state of any system featuring two stable equilibria, a qubit can be encoded into the state of a quantum system admitting a two-dimensional stable subspace. The numerical simulation of such quantum systems in the presence of realistic noise is a first step towards the design of fault-tolerant quantum computers.

Closed and open quantum systems – from Schrödinger to Lindblad

A quantum system is called *closed* if it does not interact with an outer environment, and *open* otherwise. Quantum postulates state that to any closed quantum system is associated an Hilbert space $\mathcal{H}$ such that the state of the system is described by a unit vector $|\psi\rangle \in \mathcal{H}$ and its evolution is given by the Schrödinger equation (or equivalently the Liouville equation)

$$\frac{d}{dt}|\psi\rangle = -iH|\psi\rangle \Leftrightarrow \frac{d}{dt}\rho = -i[H,\rho] \tag{2}$$

where H is a self-adjoint operator on $\mathcal{H}$ called the *hamiltonian* of the system, $\rho = |\psi\rangle\langle\psi|$ is the orthogonal projection onto $\mathrm{Span}(|\psi\rangle)$ and $[H,\rho] = H\rho - \rho H$.
The formalism can be generalized to include the case of an open quantum system: from the Schrödinger equation describing the union of an open quantum system and its environment, one can, under suitable assumptions, derive a Lindblad-type equation

$$\frac{d}{dt}\rho = -i[H,\rho] + \sum_k D[L_k](\rho) \tag{3}$$

where ρ is a *density operator*, that is a positive hermitian operator with unit trace, and $D[L](\rho) = L\rho L^\dagger - \frac{1}{2}\rho L^\dagger L - \frac{1}{2}L^\dagger L\rho$ for any operator L.
Numerical approaches must preserve the geometric properties of density operators and address the fact that the Hilbert space associated to a composite quantum system is the tensor product of the Hilbert spaces associated to each individual subsystem – the dimension of the problem thus grows *exponentially* in the number of subsystems considered.

Model order reduction vs. Intuition-based strategy

Guideline : simulating a composite systems consisting of tensor products requires efficient model order reduction strategies on each subsystem to deal with the exponential growth of the dimension.

Testbed : computation of some key coefficients in the tomography of a process describing a single idling cat-qubit, proposed in [New J. Phys. **16** 045014 (2014)]. This requires solving the following initial value problem on $\mathcal{H} = L^2(\mathbb{R},\mathbb{C})$ for a variety of initial data and parameters:

$$\frac{d}{dt}\rho = \kappa_2 D[\mathbf{a}^2 - \alpha^2](\rho) + \kappa_1 D[\mathbf{a}](\rho) + \kappa_\phi D[\mathbf{a}^\dagger\mathbf{a}](\rho) \tag{4}$$

where $\mathbf{a}$ is the annihilation operator on $\mathcal{H}$, $\alpha \in \mathbb{C}$ is a control parameter and κ_2, κ_1 and κ_ϕ are positive physical constants. We compare reference simulations using the Fock basis (requiring a basis of size $N \gg |\alpha|^2$) to the following two strategies:

Intuition-based

Observations:

1. When $\kappa_1 = \kappa_\phi = 0$, any ρ supported on $\mathrm{Span}(|\alpha\rangle, |-\alpha\rangle)$ is a fixed point of (4).
2. All operators in (4) are polynomials in $\mathbf{a}$ and $\mathbf{a}^\dagger$

Strategy: replace the Fock basis by a *shifted* Fock basis $\left(a^{\dagger n}|\pm\alpha\rangle\right)_{n\leq N_0}$ with $N_0 \ll N$.

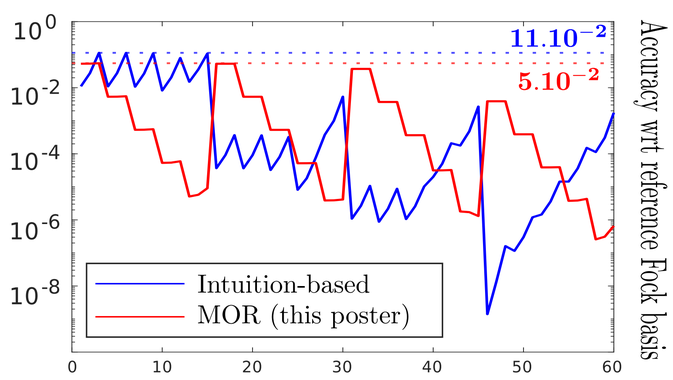
60 simulations with varying parameters

$$|\alpha|^2 \in \{2,4,6,8\}$$
$$\kappa_1 \in \{10^{-6},10^{-5},10^{-4},10^{-3},10^{-2}\}$$
$$\kappa_\phi/\kappa_1 \in \{1,2.5,10\}$$
$$\kappa_2 = 1,\ T = 4/\kappa_2$$

Model order reduction

Strategy:

1. Compute a few reference trajectories $(\rho^k(t))_{0\leq k\leq K}$ corresponding to various choices of κ_1, κ_ϕ.
2. $\rho^k(t) \simeq \sum_{r\leq R} \lambda_r |\psi_r^k(t)\rangle\langle\psi_r^k(t)|$
3. Run a PCA on the family $(|\psi_r^k(t)\rangle)_{r,k,t}$ and extract the first $N_0 \ll N$ components.



The harmonic oscillator

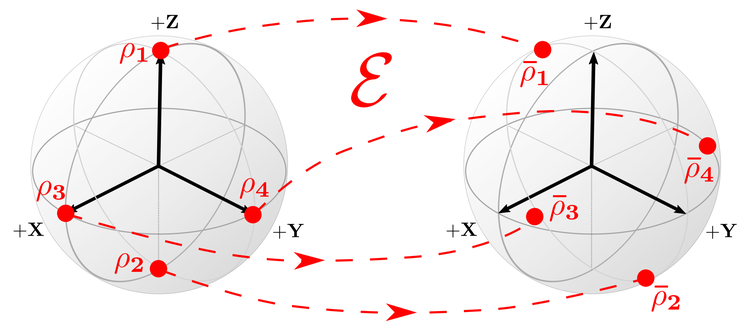
A key example is the quantum harmonic oscillator, defined by the state space $\mathcal{H} = L^2(\mathbb{R},\mathbb{C})$ and the hamiltonian $H_{ho} = \mathbf{a}^\dagger\mathbf{a} + \frac{1}{2}\mathbf{I}$ where $\mathbf{a} = \frac{1}{\sqrt{2}}(x + \partial_x)$ is called the *annihilation* operator.
The eigenvectors of H_{ho}, indexed by $n \in \mathbb{N}$, are called the *Fock states* and form an Hilbert basis of $L^2(\mathbb{R},\mathbb{C})$, with the relations $\mathbf{a}|n\rangle = \sqrt{n}|n-1\rangle$, $\mathbf{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $\mathbf{a}^\dagger\mathbf{a}|n\rangle = n|n\rangle$.
The classical strategy for the simulation of a Lindblad type equation is a Galerkin projection onto the space spanned by a finite truncation of this Fock basis.

Quantum process tomography

To characterize a linear transformation $\mathcal{E}$ of density operators on $\mathbb{C}^2$, we decompose it on a fixed basis of linear transformation:

$$\mathcal{E}(\rho) = \sum_{ij} \chi_{ij} E_i \rho E_j^\dagger \tag{1}$$

where the elementary transformations are taken from the Pauli set: $E_i \in \{I, \sigma_X, \sigma_Y, \sigma_Z\}$. The coefficients χ_{ij} above can be computed from the evolution of four initial density operators:



Numerical cost

We compare our method and other techniques of simulation of a Lindblad type equation, from the point of view of the space needed to store the solution they provide. Here, N is the truncation needed to accurately represent the solution in the Fock basis, whereas r is of the order of the rank of the solution and typically $r \ll N$.

Technique	Space cost
Fock basis	$O(N^2)$
MOR [this poster]	$O(r^2)$
Intuition-based strategy[1]	$O(r^2)$
Low-rank approximation[2]	$O(N \times r)$

[1] [arXiv:2012.04108 (2021)]
[2] [PhysRevA:87.022125 (2013)]

Conclusions

- A systematic model order reduction strategy adapted to Lindblad type equations
- Equally efficient as ad hoc state-of-the-art strategies, and outperforming brute-force approaches, on a single-qubit problem
- Intuition-free → potentially applicable to more complex settings (multi-qubit dynamics, more realistic models of a cat-qubit, other implementations of a qubit, etc.)
- Other strategies can be considered ...

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