Sample-based Hamiltonian simulation via density matrix exponentiation

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- This is an approach for performing Hamiltonian simulation by interacting a system of interest w/ program states, according to a repeated, fixed interaction.

- Before getting into it, we should review the notion of density matrix and partial trace.

- So far, we have described q. states as state vectors. Another way of doing so is via density matrices.

- Density matrix corresponding to state vector $|\psi\rangle$ is outer product

$$|\psi\rangle\langle\psi|$$

- Notice it has the benefit of removing a global phase because D.M. for $|\psi\rangle$ is $|\psi\rangle\langle\psi|$ & that for $e^{i\varphi}|\psi\rangle$ is

$$e^{i\varphi}|\psi\rangle\langle\psi|e^{-i\varphi} = |\psi\rangle\langle\psi|$$

- If we are unsure about precise state of a system, and instead only know that it is described by probabilistic ensemble $\{p(x), |\psi_x\rangle\}_x$

then corresponding density matrix is

$$\sum_x p(x)\, |\psi_x\rangle\langle\psi_x| = \rho$$

If we perform a measurement $\{\Pi_y\}_y$, outcome probability is

$$p(y) = \mathrm{Tr}[\Pi_y \rho]$$

$$= \sum_x p(x)\, \mathrm{Tr}[\Pi_y |\psi_x\rangle\langle\psi_x|]$$

$$= \sum_x p(x)\, \langle\psi_x|\Pi_y|\psi_x\rangle$$

$$= \sum_x p(x)\, \underbrace{\| \Pi_y |\psi_x\rangle \|_2^2}$$

$$\sum_x p(x)\quad p(y|x)$$

consistency w/ law of total probability

Also, ~~U~~

$|\psi\rangle \to U|\psi\rangle \Leftrightarrow |\psi\rangle\langle\psi| \to U|\psi\rangle\langle\psi|U^\dagger$ 4

Other notation we need is

partial trace.

State of two-party ~~Hilbert~~ system

is ρ_{AB}

reduced density matrix

$$\rho_A = \mathrm{Tr}_B[\rho_{AB}]$$

$$:= \sum_i (I_A \otimes \langle i|_B)\, \rho_{AB}\, (I_A \otimes |i\rangle_B)$$

state of Alice's system, used to predict outcomes of measurements on Alice's system alone

Von-Neumann equation is a consequence of Schrödinger equation

Recall that

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

(time-independent Schrö. equation)

Consider evolution of density matrix

$$i\hbar \frac{\partial}{\partial t} \left(|\psi(t)\rangle\langle\psi(t)| \right)$$

$$= i\hbar \left(|\tfrac{\partial}{\partial t}\psi(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\langle\tfrac{\partial}{\partial t}\psi(t)| \right)$$

product rule

$$= \left(i\hbar |\tfrac{\partial}{\partial t}\psi(t)\rangle \right)\langle\psi(t)| - |\psi(t)\rangle\left(\langle\tfrac{\partial}{\partial t}\psi(t)| -i\hbar\right)$$

$$= H|\psi(t)\rangle\langle\psi(t)| - |\psi(t)\rangle\langle\psi(t)| H$$

b/c conj. transpose of Schrö. eqn.

B

$$-i\hbar \left\langle \frac{\partial}{\partial t}\psi(t)\right| = \langle\psi(t)|H$$

Hermitian

$$\Rightarrow \; i\hbar \frac{\partial}{\partial t}\left(|\psi(t)\rangle\langle\psi(t)|\right)$$

$$= \left[H, |\psi(t)\rangle\langle\psi(t)|\right]$$

Now consider general

$$\rho(t) = \sum_x p_x(t)\, |\psi_x(t)\rangle\langle\psi_x(t)|$$

$$i\hbar \frac{\partial}{\partial t}\rho(t)$$

$$= i\hbar \left(\sum_x \left[\frac{\partial}{\partial t} p_x(t)\right] |\psi_x(t)\rangle\langle\psi_x(t)| \right.$$

$$\left. + \sum_x p_x(t) \frac{\partial}{\partial t}\left[|\psi_x(t)\rangle\langle\psi_x(t)|\right]\right)$$

$$= i\hbar \sum_x \left[\frac{\partial}{\partial t} p_x(t)\right] |\psi_x(t)\rangle\langle\psi_x(t)|$$

$$+ \sum_x p_x(t) \left[H, |\psi_x(t)\rangle\langle\psi_x(t)|\right]$$

$$= i\hbar \sum_x \left[\frac{\partial}{\partial t} p_x(t)\right] |\psi_x(t)\rangle\langle\psi_x(t)|$$

$$+ \left[H, \rho(t)\right]$$

for a closed system,
probabilities do not change
w/ time $\Rightarrow \frac{\partial}{\partial t} p_x(t) = 0$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t} \rho(t) = \left[H, \rho(t)\right]$$

Equivalent way to think about this:

Initial state is

$$\rho(0) = \sum_x p_x(0)\, |\psi_x(0)\rangle\langle\psi_x(0)|$$

solution of Schrö. eqn.

is

$$|\psi(t)\rangle = e^{-iHt/\hbar}\,|\psi(0)\rangle$$

$\Rightarrow$ each pure state evolves according to

$$|\psi_x(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$$

$\Rightarrow$ density matrix @ time t is

$$\rho(t) = \sum_x p_x(0)\, e^{-iHt/\hbar}|\psi(0)\rangle\langle\psi(0)|\, e^{iHt/\hbar}$$

$$= e^{-iHt/\hbar}\,\rho(0)\,e^{iHt/\hbar}$$

+ is solution of von Neumann eqn.

Idea of density matrix exponentiation:

- assume ~~a~~ Hamiltonian H is positive semidefinite & has trace one, so that it can be encoded as a density matrix, call it σ.
- then suppose we have sample access to σ, such that we can call it multiple times

then perform an interaction such that

$$\rho \otimes \sigma \otimes \cdots \otimes \sigma \rightarrow \approx e^{-i\sigma t} \rho e^{i\sigma t}$$

Consider that desired evolution for short time Δ is

$$\rho(\Delta) = e^{-i\sigma\Delta} \rho e^{i\sigma\Delta}$$

$$= (I + (-i\sigma\Delta) + O(\Delta^2)) \rho (I + i\sigma\Delta + O(\Delta^2))$$

$$= \rho - i\sigma\rho\Delta + i\rho\sigma\Delta + O(\Delta^2)$$

$$= \rho - i[\sigma, \rho]\Delta + O(\Delta^2)$$

Observe that

$$\frac{\rho(\Delta) - \rho}{\Delta} = -i[\sigma, \rho] + O(\Delta)$$

$\lim_{\Delta \to 0}$ gives von Neumann equation

$$\dot{\rho} = -i[\sigma, \rho]$$

so this kind of short time step expansion is similar to how differential equations are solved numerically, except we're considering this on a q. computer.

Now consider this

take initial state to be $\rho \otimes \sigma$ & Hamiltonian to be $SWAP \equiv F$

then

$$e^{-iF\Delta}(\rho \otimes \sigma)\, e^{iF\Delta}$$

$$= \left(I + (-iF\Delta) + O(\Delta^2)\right)(\rho\otimes\sigma)\left(I + iF\Delta + O(\Delta^2)\right)$$

$$= \rho\otimes\sigma - iF(\rho\otimes\sigma)\Delta + i(\rho\otimes\sigma)F\Delta + O(\Delta^2)$$

Now suppose we take partial trace over system 2

This implies that

$$\mathrm{Tr}_2\left[e^{-iF\Delta}(\rho\otimes\sigma)e^{iF\Delta}\right]$$

$$= \mathrm{Tr}_2[\rho\otimes\sigma] - i\,\mathrm{Tr}_2[F(\rho\otimes\sigma)]\Delta$$

$$+ i\,\mathrm{Tr}_2[(\rho\otimes\sigma)F]\Delta + O(\Delta^2)$$

$$= \rho - i\sigma\rho\Delta + i\rho\sigma\Delta + O(\Delta^2)$$

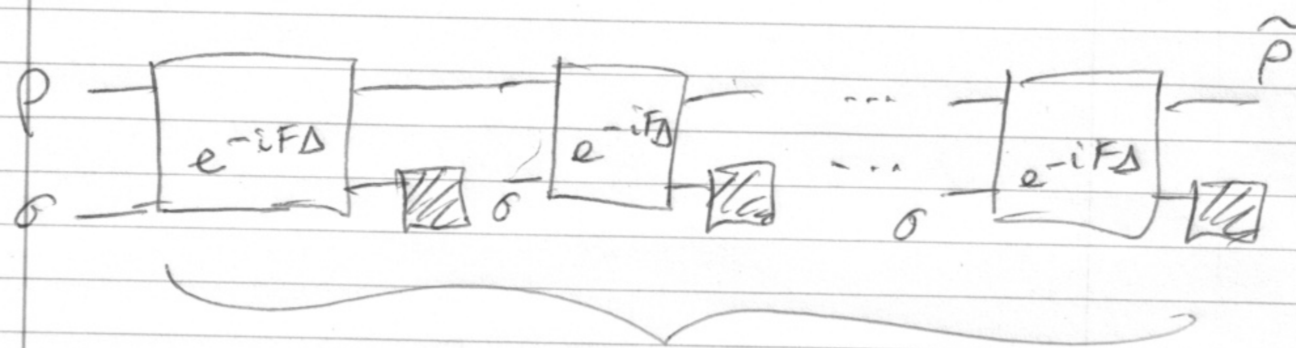
$$= \rho - i[\sigma,\rho]\Delta + O(\Delta^2)$$

$\Rightarrow$ SWAP interaction for short time & program state can simulate dynamics correctly for short time Δ.

Idea then is to pick

$$\Delta = \frac{t}{n}$$

& execute the following protocol:



n times

& we can guarantee that

$$\tilde{\rho} \approx_{\varepsilon} e^{-i\sigma t} \rho \, e^{i\sigma t}$$

if $\quad n = \dfrac{t^2}{\varepsilon}$

Proper error analysis:

Consider that

$$\mathrm{Tr}_2\left[e^{-iF\Delta}(\rho\otimes\sigma)\,e^{iF\Delta}\right]$$

$$= \mathrm{Tr}_2\Big[\Big(I - iF\Delta - \frac{I\Delta^2}{2} + o(\Delta^3)\Big)(\rho\otimes\sigma)$$

$$\Big(I + iF\Delta - \frac{I\Delta^2}{2} + o(\Delta^3)\Big)\Big]$$

b/c $\quad (-iF\Delta)^2 = -I\Delta^2$

$$= \mathrm{Tr}_2\Big[\rho\otimes\sigma - iF(\rho\otimes\sigma)\Delta + i(\rho\otimes\sigma)F\Delta$$

$$+ \underbrace{F(\rho\otimes\sigma)F}_{\sigma\otimes\rho}\Delta^2 - \rho\otimes\sigma\,\Delta^2 + o(\Delta^3)\Big]$$

$$= \rho - i[\sigma,\rho]\Delta + (\sigma-\rho)\Delta^2 + o(\Delta^3)$$

$\Rightarrow$ State @ kth step of algorithm is

$$\tilde{\rho}^{(k)} = \tilde{\rho}^{(k-1)} - i[\sigma,\tilde{\rho}^{(k-1)}]\Delta$$

$$+ (\sigma - \tilde{\rho}^{(k-1)})\Delta^2 + o(\Delta^3)$$

$\uparrow$ k-1

$+\ \tilde{\rho}^{(k-1)} = \tilde{\rho}^{(k-2)} - i[\sigma, \tilde{\rho}^{(k-2)}]\Delta$

$+ (\sigma - \tilde{\rho}^{(k-2)})\Delta^2 + o(\Delta^3)$

substitute $\tilde{\rho}^{(k-1)}$ expression into 1st line

+ get

$$\tilde{\rho}^{(k)} = \tilde{\rho}^{(k-2)} - i[\sigma, \tilde{\rho}^{(k-2)}]\Delta$$

$$+ (\sigma - \tilde{\rho}^{(k-2)})\Delta^2 + o(\Delta^3)$$

$$- i[\sigma, \tilde{\rho}^{(k-2)}]\Delta$$

$$- i[\sigma, -i[\sigma, \tilde{\rho}^{(k-2)}]]\Delta^2$$

$$+ (\sigma - \tilde{\rho}^{(k-2)})\Delta^2 + o(\Delta^3)$$

$$= \tilde{\rho}^{(k-2)} - i[\sigma, \tilde{\rho}^{(k-2)}]2\Delta$$

$$+ (\sigma - \tilde{\rho}^{(k-2)})2\Delta^2$$

$$- i[\sigma, -i[\sigma, \tilde{\rho}^{(k-2)}]]\Delta^2$$

Repeating this recursion ~~gives~~ n times starting from initial state gives

$$\tilde{\rho}^{(n)} = \tilde{\rho}^{(0)} - i\left[\sigma, \tilde{\rho}^{(0)}\right] n\Delta$$

$$+ \left(\sigma - \tilde{\rho}^{(0)}\right) n\Delta^2$$

$$\underbrace{-i\left[\sigma, -i\left[\sigma, \tilde{\rho}^{(0)}\right]\right]}_{-\left[\sigma,\left[\sigma, \tilde{\rho}^{(0)}\right]\right]} \left(1 + 2 + \cdots + n-1\right)\Delta^2 + O(\Delta^3)$$

$$1 + 2 + \cdots + n-1 = \frac{n(n-1)}{2}$$

Ideal evolution is , for time $t = n\Delta$

$$e^{-i\sigma n\Delta} \rho \, e^{i\sigma n\Delta}$$

$$= \left(I - i\sigma n\Delta - \frac{\sigma^2 n^2 \Delta^2}{2} + O(\Delta^3)\right) \rho \left(I + i\sigma n\Delta - \frac{\sigma^2 n^2 \Delta^2}{2} + O(\Delta^3)\right)$$

$$= \rho - i[\sigma, \rho] n\Delta - \frac{1}{2}[\sigma, [\sigma, \rho]] n^2\Delta^2 + O(\Delta^3)$$

then subtracting ideal from actual gives

$$(\sigma - \tilde{\rho}^{(0)}) n\Delta^2 - [\sigma, [\sigma, \tilde{\rho}^{(0)}]] n\Delta^2 + O(\Delta^3)$$

$$= O(n\Delta^2) = O\left(\frac{t^2}{n}\right) \qquad \Delta = t/n$$

$\Rightarrow$ if desired error is ε then pick $\varepsilon = \frac{t^2}{n}$

$$\Rightarrow n = \frac{t^2}{\varepsilon}$$

$$\Rightarrow n = O\left(\frac{t^2}{\varepsilon}\right)$$