Quantum simulation on a random tensor network

February 1, 2022

1 Differentiating single step time evolution

The m site Rydberg Hamiltonian is

$$H_{\text{Rydberg}} = \sum_{i,j=1,i>j}^{m} \frac{C}{|r_i - r_j|^6} n_i n_j + \Omega(t) \sum_{i=1}^{m} \frac{1}{2}\sigma_i^x + \Delta(t) \sum_{i=1}^{m} n_i \tag{1}$$

For simplicity, we consider the following general representation of a time-space dependent Hamiltonian with k terms

$$H = \sum_{k=1}^{K} c_k O_k \tag{2}$$

where c_k can be dependent on a set of parameters like locations $r_1, r_2, \ldots, r_m$, and pulses $\Omega(t)$ and $\Delta(t)$.

1.1 The ODE version

In each step of the ODE solver, it performs the following update

$$|\psi'\rangle = (1 - iH\Delta t)|\psi\rangle \tag{3}$$

We derive the backward rules for the gradients by inspecting the following equations

$$\begin{aligned} \overline{\mathcal{L}}\delta\mathcal{L} &= \overline{|\psi'\rangle} \circ \delta|\psi'\rangle \\ &= \sum_k \overline{c_k}\delta c_k + \overline{|\psi\rangle} \circ \delta|\psi\rangle + \overline{\Delta t}\delta\Delta t \end{aligned} \tag{4}$$

where $\circ$ is the Hadamard product applied on real numbers, note a complex number in computer is composed of two real numbers. The above euqations has a more elegant linear algebra version as the following.

$$\begin{aligned} \overline{\mathcal{L}}\delta\mathcal{L} &= \overline{\langle\psi'|}\delta|\psi'\rangle \\ &= \sum_k \overline{c_k}\delta c_k + \overline{\langle\psi|}\delta|\psi\rangle + \overline{\Delta t}\delta\Delta t \end{aligned} \tag{5}$$

where we have used $\langle\psi|$ to represent the hermitian conjugate of $|\psi\rangle$.

$$\delta|\psi'\rangle = -i\sum_k \delta c_k O_k \Delta t|\psi\rangle - iH\delta\Delta t|\psi\rangle + (1 - iH\Delta t)\delta|\psi\rangle \tag{6}$$

By observing Eq. (5) and Eq. (6), one can see

$$\overline{\langle\psi|} = \overline{\langle\psi'|}(1 - iH\Delta t) \tag{7}$$

$$\overline{c_k} = \Re\left[-i\Delta t\overline{\langle\psi'|}O_k|\psi\rangle\right] \tag{8}$$

$$\overline{\Delta t} = \Re\left[-i\overline{\langle\psi'|}H|\psi\rangle\right] \tag{9}$$

After a step, a normalization procedure might be called on the wave functions, this is trivial so that we do not discuss it at this stage.

1.2 The `expmv` version

To differentiate the time evolution directly, one can use the Taylor expansion

$$\begin{aligned}|\psi'\rangle &= e^{-iHt}|\psi\rangle \\ &= \sum_{n=0}^{\infty}\frac{(-it)^n H^n}{n!}|\psi\rangle\end{aligned} \tag{10}$$

Similarly, we have

$$\delta|\psi'\rangle = e^{-iHt}\delta|\psi\rangle + \sum_{n=0}^{\infty}\frac{(-it)^n\delta(H^n)}{n!}|\psi\rangle + \left(e^{-iH(t+\delta t)} - e^{-iHt}\right)|\psi\rangle \tag{11}$$

$$\overline{\langle\psi|} = \overline{\langle\psi|}e^{-iHt}\delta \tag{12}$$

$$\bar{t} = \overline{\langle\psi'|} - iHe^{-iHt}|\psi\rangle \tag{13}$$

$$\overline{c_k} = \sum_n \frac{(-it)^n}{n!}\sum_{p=0}^{n-1}\overline{\langle\psi'|}H^p O_k H^{n-p-1}|\psi\rangle \tag{14}$$

2 How to reverse the time evolution

1. Since the time evolution of a Hamiltonian is sympletic, one can reverse it by doing inverse time evolution.
2. For the cases reversibility is not guarented, one can use treeverse algorithm.

References