Quantum simulation on a random tensor network

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[**JG: This is how you make a comment. Hi**] [**MD: Hi**], [**RG: Hi**].

1 The Dirac-Frenkel's variational principle

We have a Hamiltonian for a quantum system with K terms.

$$H = \sum_{k=1}^{K} \prod_{i=1}^{n} o_i^k \tag{1}$$

where n is the system size and o_i^k is a local operator on site i. We can see each term is a product of local operators. Let $\psi(\theta)$ be the ansatz of wave functions, to obtain the dynamics of the parameters. We treat $x \equiv \frac{\partial \theta}{\partial t}$ as the variational parameters, and set the goal is to minimize [1]

$$\mathcal{L} = \left\| i\frac{\partial \psi}{\partial \theta} x - H\psi \right\|^2 . \tag{2}$$

At the extrema, we have $\frac{\partial \mathcal{L}}{\partial x} = 0$. That is

$$0 = (-i\frac{\partial \psi^*}{\partial \theta})(i\frac{\partial \psi}{\partial \theta}x - H\psi) + (-ia\frac{\partial \psi^*}{\partial \theta} - \psi^* H)(i\frac{\partial \psi}{\partial \theta}) \tag{3}$$

$$= \frac{\partial \psi^*}{\partial \theta}\frac{\partial \psi}{\partial \theta}x + i\frac{\partial \psi^*}{\partial \theta}H\psi + x\frac{\partial \psi^*}{\partial \theta}\frac{\partial \psi}{\partial \theta} - i\psi^* H\frac{\partial \psi}{\partial \theta} \tag{4}$$

Finally, we arrive at the Dirac-Frenkel's variational principle by taking the first two terms [**JG: Because the wave function is analytic complex valued function, when the real parts of two functions are the same, their complex components are the same too.**]

$$\frac{\partial \psi^*}{\partial \theta}\frac{\partial \psi}{\partial \theta}x = -i\frac{\partial \psi^*}{\partial \theta}H\psi \tag{5}$$

[**JG: In tensor network representation, we can normalize tensor networks easily, so we do not need to go to the unnormalized prepresentation.**]

1.1 The automatic differentiation approach

The first term can be computed as

$$\begin{aligned} \mathcal{L}_1(\theta, \theta') &= \psi(\theta)^* \psi(\theta'), \\ \mathcal{G}_1(\theta) &= \frac{\partial \mathcal{L}_1(\theta, \theta')}{\partial \theta'} x, \\ \frac{\partial \psi^*}{\partial \theta} \frac{\partial \psi}{\partial \theta} x &= \frac{\partial \mathcal{G}_1(\theta)}{\partial \theta} \Big|_{\theta=\theta'} \end{aligned} \tag{6}$$

where $\psi(\theta) = \texttt{normalize}(\texttt{tensornetwork}(\theta))$. The second term can be computed as

$$\begin{aligned} \mathcal{L}_2(\theta) &= -i\psi(\theta)^* H \psi \\ -i \frac{\partial \psi^*}{\partial \theta} H \psi &= \frac{\partial \mathcal{L}_2(\theta)}{\partial \theta} \end{aligned} \tag{7}$$

1.2 Time and space complexity

Let us denote the time complexity of contracting the overlap $\psi^*\psi$ as 1. Eq. (6) can be evaluated by reverse differentiating first order gradient program G_1. Obtaining the gradient of the program through back propagation only introduces a constant overhead, and let us denote this constant as c. Then the overhead of obtaining the Hessian is c^2. The time to evaluate expectation values of all terms in the Hamiltonian in Eq. (7) is K. Hence the overall time overhead is $K + c^2$. The space overhead is propotional to the size of intermediate contraction results of tensor networks, which is dominated by the largest tensors.

References

[1] J Broeckhove, L Lathouwers, E Kesteloot, and P Van Leuven. On the equivalence of time-dependent variational principles. *Chemical physics letters*, 149(5-6):547–550, 1988.