Brief Report

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Augest 2019

1 Optimization Problem

let $\lambda_1 \dots \lambda_m$ be set of free degrees of Hamiltonian, $|\phi_0\rangle$ the ground state and $|\psi\rangle$ the target state.

formally, the problem can be formulated by this equation

$$H^*(\lambda_1 \dots \lambda_m), t^* = \underset{\lambda_1..\lambda_m, t}{\arg\max}\, \mathcal{F}(e^{iH(\lambda_1 \dots \lambda_m)t} |\phi_0\rangle, |\psi\rangle)$$

where $\mathcal{F}(.,.)$ is fidelity.

specifically, we are focusing on a Hisenberg model, therefore

$$H(J_1 \dots J_{N-1}, B_1 \dots B_N) = \sum_{i=1}^{N-1} J_i(X_i X_{i+1} + Y_i Y_{i+1}) + \sum_{i=1}^{N} B_i(1 - Z_i)$$

In this case, by multiplying each degrees by α, and dividing t by α result remains the same, therefore we can substitute t with t_0.

$$H^*(J_1 \dots J_{N-1}, B_1 \dots B_N) = \underset{J_1 \dots J_{N-1}, B_1 \dots B_N}{\arg\max} \mathcal{F}(e^{iHt_0} |\phi_0\rangle, |\psi\rangle) \tag{1}$$

2 Minimum Guaranteed Fidelity

for any method for estimating states (that estimates $|\phi\rangle$ with $\mathrm{Est}[|\phi\rangle]$, we can define a “minimum guaranteed fidelity” (MGF) that

$$\mathcal{F}(|\phi\rangle, \mathrm{Est}[|\phi\rangle]) \geq \mathrm{MGF}$$

in order to find MGF empirically, we define a mapping $f : \mathbb{R}^{2N} \to \mathcal{H}$ with $\dim \mathcal{H} = N$ as

$$f(\vec{\mathbf{v}}) := \sum_{i=1}^{N} (v_{2i} + iv_{2i+1}) |i\rangle$$

Lemma 1. *for two arbitrary vectors $\vec{\mathbf{v}}$ and $\vec{\mathbf{v}'}$ in $\mathbb{R}^{2N}$*

$$\mathcal{F}(f(\vec{\mathbf{v}}), f(\vec{\mathbf{v}'})) \geq \vec{\mathbf{v}} \cdot \vec{\mathbf{v}'}$$

now we choose a set of k equidistributed points on a 2N-d unit hypersphere called P.

for an arbitrary point $\vec{\mathbf{x}}$ on sphere, exists $\vec{\mathbf{t}} \in P$ that $\forall \vec{\mathbf{p}} \in P - \{\vec{\mathbf{t}}\}\ \ \vec{\mathbf{t}} \cdot \vec{\mathbf{x}} > \vec{\mathbf{t}} \cdot \vec{\mathbf{p}}$

then by mapping to hilbert space

$$S := \{f(\vec{\mathbf{p}}) \mid \vec{\mathbf{p}} \in P\}$$

$$d := \min_{\vec{\mathbf{x}} \in P} \max_{\vec{\mathbf{y}} \in P - \{\vec{\mathbf{x}}\}} \vec{\mathbf{x}} \cdot \vec{\mathbf{y}}$$

$$\forall \left|\phi\right\rangle \in \mathcal{H} \ \ \exists \left|t\right\rangle \in S \ \ \mathcal{F}(\left|\phi\right\rangle, \left|t\right\rangle) \geq d$$

We know from Fubini-Study metric that for three arbitrary states $|a\rangle$, $|b\rangle$ and $|c\rangle$

$$\arccos \sqrt{\mathcal{F}(\left|a\right\rangle, \left|c\right\rangle)} \geq \arccos \sqrt{\mathcal{F}(\left|a\right\rangle, \left|b\right\rangle)} + \arccos \sqrt{\mathcal{F}(\left|b\right\rangle, \left|c\right\rangle)}$$

now defining these

$$E_{\mathcal{H}} := \{\mathrm{Est}[\left|\phi\right\rangle] \mid \ \left|\phi\right\rangle \in \mathcal{H}\}$$

$$E_S := \{\mathrm{Est}[\left|s\right\rangle] \mid \ \left|s\right\rangle \in S\}$$

$$f_{\min} := \min_{\left|s\right\rangle \in S} \mathcal{F}(\left|s\right\rangle, \mathrm{Est}[\left|s\right\rangle])$$

and for all $|\phi\rangle$

$$\mathcal{F}(\left|\phi\right\rangle, \mathrm{Est}[\left|\phi\right\rangle]) = \max_{\left|e\right\rangle \in E_{\mathcal{H}}} \mathcal{F}(\left|\phi\right\rangle, \left|e\right\rangle)$$

we know $E_S \subseteq E_{\mathcal{H}}$

$$\begin{aligned}
\mathcal{F}(\left|\phi\right\rangle, \mathrm{Est}[\left|\phi\right\rangle]) &\geq \max_{\left|s\right\rangle \in S} \mathcal{F}(\left|\phi\right\rangle, \mathrm{Est}[\left|s\right\rangle]) \\
&\geq \max_{\left|s\right\rangle \in S} \cos^2 \left(\arccos \sqrt{\mathcal{F}(\left|\phi\right\rangle, \left|s\right\rangle)} + \arccos \sqrt{\mathcal{F}(\left|s\right\rangle, \mathrm{Est}[\left|s\right\rangle])} \right) \\
&\geq \max_{\left|s\right\rangle \in S} \cos^2 \left(\arccos \sqrt{\mathcal{F}(\left|\phi\right\rangle, \left|s\right\rangle)} + \arccos \sqrt{f_{\min}} \right) \\
&\geq \cos^2(\arccos \sqrt{d} + \arccos \sqrt{f_{\min}}) = (\sqrt{d}\sqrt{f_{\min}} - \sqrt{1-d}\sqrt{1-f_S})^2
\end{aligned}$$

3 Numerical Optimization

3.1 N-sector Subspace

We know that $[H, S_{\text{total}}] = 0$ where S_{total} is total spin operator. therefore, we can rewrite H as a parameteric matrix in each N-sector subspace with basis $e_1 \ldots e_m$

$$H_{ij} = \langle e_i | H | e_j \rangle$$

And for the sake of simplicity we can assume ground state is $|e_1\rangle$

Now eq. 1 as a parameteric optimization problem, can be solved approximately for any target state using gradient-descent method by a deep-learning framework. This approach is the same as what Innocenti. et. al. did for gate construction.

the result of solving eq. 1 for a target state such as $|\phi\rangle$, will give us a Hamiltonian, therefore, we can define $\mathrm{Est}[|\phi\rangle] = e^{iH^*t}$ and consequently MGF.

Note that due to randomness in initialization of this optimization method, which leads to sub-optimal results, we repeat the optimization for each target multiple times and report the best result.

4 Results

for reporting results, we define

$$\bar{f} := \frac{\sum_{|s\rangle \in S} \mathcal{F}(|s\rangle, \mathrm{Est}[|s\rangle])}{|S|}$$

$\dim \mathcal{H}$	$\lvert S\rvert$	d	$\bar{f}$	$f_{\min}$	MGF
2	2560	0.980	0.99995	0.996	0.959
3	13734	0.955	0.99570	0.944	0.810
4	22599	0.921	0.96058	0.621	0.340

Table 1: one-sector subspace

Appendix

proof of Lemma 1:

$$\begin{aligned}
\langle f(v)|f(v')\rangle &= \sum_{i=1}^{N} f(v')_i^* f(v)_i = \sum_{i=1}^{N} (v_{2i} - iv_{2i+1})(v'_{2i} + iv'_{2i+1}) \\
&= \sum_{i=1}^{N} v_{2i}v'_{2i} + v_{2i+1}v'_{2i+1} + \sum_{i=1}^{N} i(v_{2i}v'_{2i+1} - v'_{2i}v_{2i+1}) \\
&= \vec{\mathbf{v}} \cdot \vec{\mathbf{v}'} + \sum_{i=1}^{N} i(v_{2i}v'_{2i+1} - v_{2i}v_{2i+1} + v_{2i}v_{2i+1} - v'_{2i}v_{2i+1})
\end{aligned}$$

defining $I \in \mathbb{R}$ as

$$\langle f(v)|f(v')\rangle = \vec{\mathbf{v}} \cdot \vec{\mathbf{v}'} + iI$$

$$\begin{aligned}
\mathcal{F}(|f(v)\rangle, |f(v')\rangle) = |\langle f(v)|f(v')\rangle| &= \sqrt{(\vec{\mathbf{v}} \cdot \vec{\mathbf{v}'})^2 + I^2} \\
&\geq \vec{\mathbf{v}}.\vec{\mathbf{v}'}
\end{aligned}$$