Thu, June 1, 2023

Goal : Find ground state of H

Suppose $H = \sum_j a_j L_j$

where L_j are k-local Pauli terms and $\|a\| = 1$.

Ref : "Determining a local Hamiltonian from a single eigenstate

Sps we know v is any eigenstate of H.

Let $M^{(v)} \equiv [M_{ij}] = \frac{1}{2}\langle \{L_i, L_j\}\rangle_v - \langle L_i\rangle_v \langle L_j\rangle_v$

where $\{L_i\}$ a basis of k-local Pauli operators.

- Then M has a non-degenerate zero eigenvalue

(Note $M \succeq 0$). $0 = \lambda_0 < \lambda_1 < \dots$, $\{w_0, w_1, \dots\}$

$H = \sum (w_0)_i L_i$

Denote v^* is ground state of H.

$H' :=$ approx of H

$= \sum_j w_j L_j$

$$\Rightarrow \quad \min \sum_j |a_j - w_j|^2 \quad (\min \|H - H'\|^2)$$

$$\text{st.} \begin{cases} M^{(v)} \cdot w = 0 \\ v = \text{ground state of } H' \end{cases}$$

Algorithm to find v^*

- Start w/ any eigenstate v_k of H'_{k-1}

Start v_0 = ground state of H'_{-1} = a commuting part of H ("Fast Partitioning of Pauli Strings into Commuting Families ...")

$\downarrow$

$M^{(v_k)}$

$\downarrow$

$|\mu| \ll 1$

- $w_k = w_{k-1} - \mu \nabla \|a - w\|^2 \Big|_{w = w_{k-1}}$

constrained to $M^{(v_k)} w_k = 0$

$\|a - w\| \simeq 0$, $H'_k \simeq H$

($w_k \sim$ perturbation of w_{k-1})

$\downarrow$

$H'_k = \sum_j (w_k)_j L_j$

$\hookrightarrow$ Next iteration : $v_{k+1} \sim$ ground state of H'_k

$v_k \sim$ ground state of H'_{k-1}

$H'_k \sim$ perturbation of H'_{k-1} $\qquad H'_k = H'_{k-1} + \mu V$

$|\psi(\theta_{k+1})\rangle \equiv v_{k+1} \xleftarrow{\text{perturbation theory}} v_k \equiv |\psi(\theta_k)\rangle$

$$H = H_0 + \lambda V \qquad (|\lambda| \ll 1)$$

$E_n^{(0)}$: eigenvalue of H_0 , eigenstate $|n^{(0)}\rangle$

E_n : eigen value of H , eigenstate $|n\rangle$

$$E_n = \underline{E_n^{(0)}} + \underline{\langle n^{(0)}|\lambda V|n^{(0)}\rangle} + \underbrace{\sum_{k\neq n} \frac{|\langle n^{(0)}|\lambda V|k^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}}}_{\text{correction}} + \cdots \qquad |E_n^{(0)} - E_k^{(0)}| < \delta$$

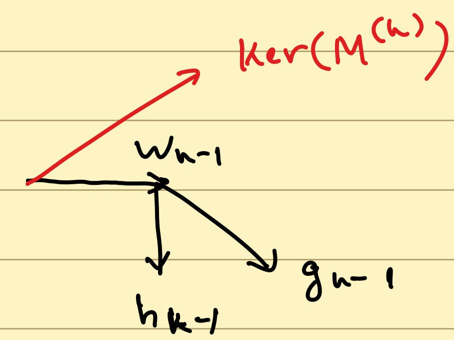
$$|n\rangle = |n^{(0)}\rangle + \sum_{k\neq n} |k^{(0)}\rangle \cdot \frac{|\langle n^{(0)}|\lambda V|k^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}} + \cdots$$

$$v_k \equiv |\psi(\vec{\theta}_k)\rangle$$

$$w_k = w_{k-1} - \nabla \|w - a\|^2$$
$$\text{st.} \quad M w_k = 0$$

$$g_{k-1} = \nabla \|w - a\|^2 \Big|_{w = w_{k-1}}$$
$$g_{k-1} = \alpha w_{k-1} + \beta n_{k-1} \quad ; \quad \|n_{k-1}\| = 1$$

$$w_k = a w_{k-1} + b n_{k-1}$$
$$M w_k = a M w_{k-1} + b M n_{k-1}$$



$$\mathcal{L}(w,\lambda) = \|a - w\|^2 + \lambda^T M w$$
$$= \|a\|^2 - 2 a\cdot w + \|w\|^2 + \lambda M w$$

$$\nabla_{w,\lambda} \mathcal{L} = \begin{bmatrix} 2(w-a) + M\lambda \\ Mw \end{bmatrix}$$

$$\text{Want} \quad \nabla \mathcal{L} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\rightarrow \quad \text{Min} \; f(w,\lambda) = \|2(w-a) + M\lambda\|^2 + \|Mw\|^2$$
$$= 4\|w-a\|^2 + 4(w-a)^T M\lambda + \|M\lambda\|^2 + \|Mw\|^2$$

$$\nabla_w f = 8(w-a) + 4M\lambda + 2M^T M w$$
$$\nabla_\lambda f = 4M(w-a) + 2M^T M\lambda$$