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Variational Q. Algorithms

For applications, we are interested in the minimum eigenvalue of a Hermitian matrix.

In physics, H is a Hamiltonian which is an energy observable.

To determine the energy of a state $|\psi\rangle$, we calculate

$$\langle\psi|H|\psi\rangle = \mathrm{Tr}\left[H\,|\psi\rangle\langle\psi|\right]$$

Then the minimum energy is given by

$$\min_{|\psi\rangle} \langle\psi|H|\psi\rangle$$

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minimum energy is often called ground state energy. Helps to predict properties of the system.

Math background

Eigenvector $|\psi_i\rangle$ of H is such that

$$H|\psi_i\rangle = \lambda_i |\psi_i\rangle$$

eigenvalue

can write H as

$$H = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$$

then $\langle\psi|H|\psi\rangle = \langle\psi| \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|\psi\rangle$

$$= \sum_i \lambda_i \langle\psi|\psi_i\rangle\langle\psi_i|\psi\rangle$$

$$= \sum_i \lambda_i |\langle \psi | \psi_i \rangle|^2$$

Since $|\langle \psi | \psi_i \rangle|^2 \geq 0$
it follows that

$$\sum_i \lambda_i |\langle \psi | \psi_i \rangle|^2$$

$$\geq \sum_i \lambda_{min} |\langle \psi | \psi_i \rangle|^2$$

$$= \lambda_{min} \sum_i |\langle \psi | \psi_i \rangle|^2$$

$$= \lambda_{min} \sum_i \langle \psi | \psi_i \rangle \langle \psi_i | \psi \rangle$$

$$= \lambda_{min} \langle \psi | \sum_i |\psi_i \rangle \langle \psi_i | \, | \psi \rangle$$

$$= \lambda_{min} \langle \psi | \psi \rangle$$

$$= \lambda_{min}$$

Thus, we have shown that

$$\lambda_{min} \leq \langle\psi|H|\psi\rangle \qquad \forall|\psi\rangle$$

called variational principle

inequality saturated by picking

$|\psi\rangle = |\psi_{min}\rangle$ i.e. eigenvector

w/ $H|\psi_{min}\rangle = \lambda_{min}|\psi_{min}\rangle$

b/c

$$\langle\psi_{min}|H|\psi_{min}\rangle$$

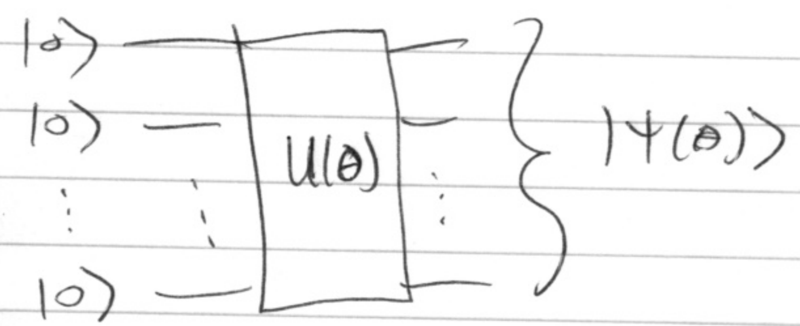
$$= \langle\psi_{min}|\sum_i \lambda_i |\psi_i\rangle\langle\psi_i| \; |\psi_{min}\rangle$$

$$= \sum_i \lambda_i |\langle\psi_{min}|\psi_i\rangle|^2$$

$$= \sum_i \lambda_i \delta_{i,min} = \lambda_{min}$$

Idea of variational eigensolver:
try to find $|\psi_{min}\rangle$ by using a q. computer!

generate $|\psi(\theta)\rangle$ by running



Then use $|\psi(\theta)\rangle$ state to estimate $\langle\psi(\theta)|H|\psi(\theta)\rangle$

How to do this?

Suppose that

$$H = \sum_{z_1,\ldots,z_m \in \{0,\ldots,3\}} \alpha_{z^m} \overbrace{\sigma_{z_1} \otimes \sigma_{z_2} \otimes \cdots \otimes \sigma_{z_m}}^{\text{string of Pauli matrices}}$$

where $\alpha_{z^m} = \alpha_{z_1,\ldots,z_m} \in \mathbb{R}$

Then it follows that

$$\langle \psi(\theta) | H | \psi(\theta) \rangle$$

$$= \sum_{z_1,\ldots,z_m \in \{0,1,\ldots,3\}} \alpha_{z^m} \underbrace{\langle \psi(\theta) | \sigma_{z_1} \otimes \sigma_{z_2} \otimes \cdots \otimes \sigma_{z_m} | \psi(\theta) \rangle}$$

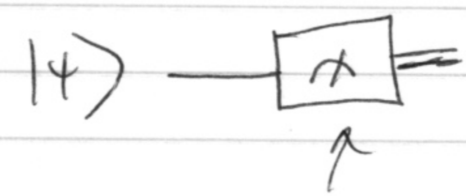
So if we can estimate $\forall z^m$ for which α_{z^m} is non-zero, then we can estimate $\langle \psi(\theta) | H | \psi(\theta) \rangle$

How to estimate?

Consider simple example of estimating

$\langle\psi|\sigma_z|\psi\rangle$ for a single qubit

Do it this way



computational basis measurement
i.e. $\{|0\rangle\langle 0|, |1\rangle\langle 1|\}$

~~If outcome~~

Consider that $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$,

so that

$$\langle\psi|\left(|0\rangle\langle 0| - |1\rangle\langle 1|\right)|\psi\rangle$$

$$= \left|\langle\psi|0\rangle\right|^2 - \left|\langle\psi|1\rangle\right|^2$$

In one run of experiment, if $|0\rangle\langle 0|$ outcome occurs, ~~we~~ set $Z_1 = +1$

If $|1\rangle\langle 1|$ outcome occurs, write down $Z_1 = -1$

keep doing this n times & get

$$Z_1, \ldots, Z_n$$

output estimate of $\langle\psi|\sigma_z|\psi\rangle$ as

$$\overline{Z^n} = \frac{Z_1 + \cdots + Z_n}{n}$$

By Hoeffding inequality, in order to have

$$\Pr\left\{ \left| \overline{Z^n} - \langle\psi|\sigma_z|\psi\rangle \right| \leq \varepsilon \right\} \geq 1 - \delta$$

It suffices to pick

$$n \geq \frac{2}{\varepsilon^2} \log\left(\frac{2}{\delta}\right)$$

Tells us the # of times we need to run the experiment to get a good [illegible]

How to estimate $\langle\psi|\sigma_x|\psi\rangle$?

Execute 

Set $Z_1 = +1$ if $|0\rangle\langle 0|$ occurs

& $Z_1 = -1$ if $|1\rangle\langle 1|$ occurs

Then running n times & calculating $\frac{Z_1 + \dots + Z_n}{n}$

gives ε-accurate estimate w/ success prob. $\geq 1-\delta$

How to estimate $\langle\psi|\sigma_y|\psi\rangle$?

Execute 

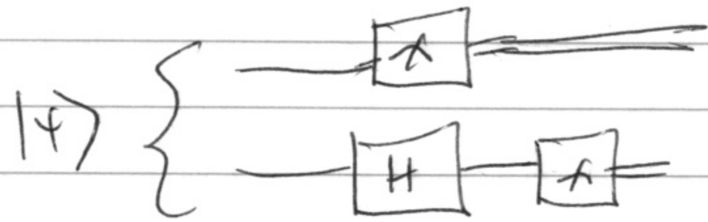
where $H_y = |0\rangle\langle +y| + |1\rangle\langle -y|$

& same thing

How to estimate for two qubits?

$$\langle\psi|\, \sigma_z \otimes \sigma_x \,|\psi\rangle$$

Execute



If "0" occurs on 1st then set

$$Z_{1,1} = +1$$

If "1" occurs on 1st then set

$$Z_{1,1} = -1$$

If "0" occurs on second then set

$$Z_{1,2} = +1$$

If "1" occurs on second, then set

$$Z_{1,2} = -1$$

Set $Z_1 = \cancel{Z}_{1,1} \cdot Z_{1,2}$

repeat n times + calculate $\dfrac{Z_1 + \dots + Z_n}{n}$ as before

Why does this work?

Consider that

$$\sigma_Z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

$$\sigma_X = |+\rangle\langle +| - |-\rangle\langle -|$$

so that

$$\sigma_Z \otimes \sigma_X = \left(|0\rangle\langle 0| - |1\rangle\langle 1|\right) \otimes \left(|+\rangle\langle +| - |-\rangle\langle -|\right)$$

$$= |0+\rangle\langle 0+| - |1+\rangle\langle 1+| - |0-\rangle\langle 0-|$$
$$+ |1-\rangle\langle 1-|$$

$$\Rightarrow \langle \psi | \sigma_Z \otimes \sigma_X | \psi \rangle$$

$$= |\langle \psi | 0+\rangle|^2 - |\langle \psi | 1+\rangle|^2$$
$$- |\langle \psi | 0-\rangle|^2 + |\langle \psi | 1-\rangle|^2$$

$$= \sum_{z_{1,1},\, z_{1,2} \in \{+1,-1\}} z_{1,1} \cdot z_{1,2} \; P_r(z_{1,1}, z_{1,2})$$

So the idea is to calculate

estimates

$$\tilde{E}^{n}_{z^m} \approx \langle \psi | \sigma_{z_1} \otimes \sigma_{z_2} \otimes \cdots \otimes \sigma_{z_m} | \psi \rangle$$

& than output estimate of

$\langle \psi | H | \psi \rangle$ as

$$\sum_{z^m} \alpha_{z^m} \tilde{E}^{n}_{z^m}$$

again guaranteed that

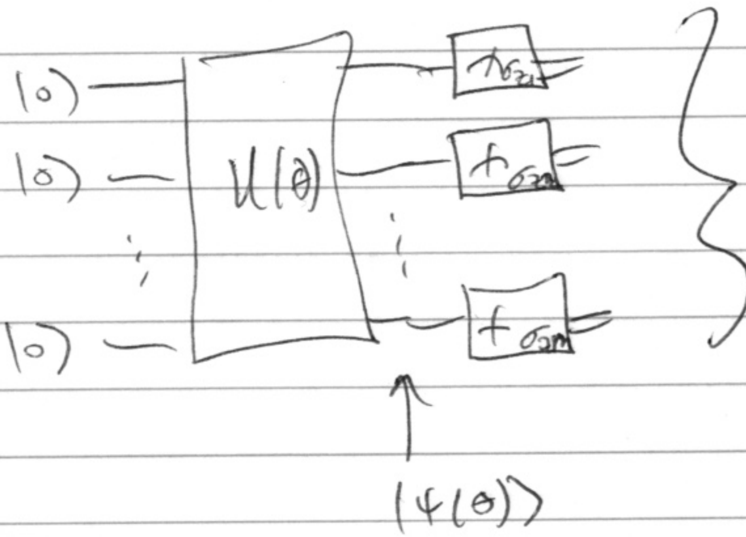
$$\Pr\left[\left| \sum_{z^m} \alpha_{z^m} \tilde{E}^{n}_{z^m} - \langle \psi | H | \psi \rangle \right| \le \varepsilon \right]$$

$\ge 1-\delta$ as long as

$$n \ge \frac{\left(\sum_{z^m} |\alpha_{z^m}| \right)^2}{2\varepsilon^2} \log\left(\frac{2}{\delta}\right)$$

Idea behind VQE:

Prepare $|\psi(\theta)\rangle$ using



repeat many times to estimate $\underbrace{\langle\psi(\theta)|H|\psi(\theta)\rangle}_{\text{called cost function}}$

Now use a classical computer to modify θ, to try & make $\langle\psi(\theta)|H|\psi(\theta)\rangle$ smaller

repeat the whole procedure some number of times until convergence occurs.

Two questions remain:

1) How to choose $U(\theta)$?

2) How to ~~minimize~~ choose θ when repeating, in order to minimize $\langle \psi(\theta) | H | \psi(\theta) \rangle$?