FYS5419, APRIL 17, 2023

$$R_x = e^{-i\theta/2\,\sigma_x} = R_x(\theta)$$

rotation around x-axis

$$R_x(\theta) = \mathbb{1}\cdot\cos\theta/2 - i\sigma_x \sin\frac{\theta}{2}$$

$$R_y = R_y(\phi) = e^{-i\phi/2\,\sigma_y}$$

$$= \mathbb{1}\cdot\cos\frac{\phi}{2} - i\sigma_y \sin\phi/2$$

For one-qubit state, we have a general qubit state on the Bloch sphere

$$|\psi\rangle = R_x(\theta)R_y(\phi)|0\rangle$$

$$H_0|0\rangle = E_1|0\rangle$$

$$H_0|1\rangle = E_2|1\rangle$$

$$E_1 < E_2$$

$$\hat{\theta}, \hat{\phi} = \underset{\theta,\phi \in \mathbb{R}}{\operatorname{argmin}} \langle\psi|H|\psi\rangle$$

we will use gradient descent to find the optimal values

$$\langle\psi|H|\psi\rangle = \langle 0|[R_x(\theta)R_y(\phi)]^{\dagger} H$$

$$\times\; R_x(\theta)R_y(\phi)|0\rangle$$

$$|\psi\rangle = |0\rangle - \boxed{R_x(\theta)} - \boxed{R_y(\phi)} -$$

$R_x, R_y \Rightarrow R_i = R_i(\phi)$

$i = x, y, z$

$$R_i(\phi) = e^{-i\,\phi/2\,\sigma_i} \Rightarrow$$

$$R(\phi) = e^{-i\phi G}$$

$$\left(G = \frac{\sigma_x}{2}, \frac{\sigma_y}{2}, \ldots \right)$$

$$\frac{\partial R}{\partial \phi} = -iG\,e^{-i\phi G} = -iG R(\phi)$$

$$\langle\psi|H|\psi\rangle = \langle 0|R^{+} H R|0\rangle$$

$$|\psi\rangle = R|0\rangle$$

$$\frac{\partial}{\partial\phi}\left[\langle 0|R^{+} H R|0\rangle\right]$$

$$= \langle 0|R^{+} H \left(\frac{\partial}{\partial\phi} R\right)|0\rangle + h.c.$$

$$= \langle 0|R^{+} H (-iG) R|0\rangle + h.c.$$

$$= \langle\psi|H(-iG)|\psi\rangle + h.c.$$

$$\langle\psi|A^{\dagger}BC|\psi\rangle + h.c.$$

$$= \frac{1}{2}\Big[\langle\psi|(A+C)^{\dagger}B(A+C)|\psi\rangle$$

$$- \langle\psi|(A-C)^{\dagger}B(A-C)|\psi\rangle\Big]$$

$$A = \mathbb{1} \qquad B = H$$

$C = -i r^{-1} G$ we have assumed that G has two distinct eigenvalues $\pm r$

$$\Big[\ \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\ \Big]$$

$$\frac{\partial}{\partial\phi}\langle H\rangle = \frac{r}{2}\Big[\langle\psi|(\mathbb{1}-i r^{-1}G)^{\dagger}$$

$$\times H(\mathbb{1}-i r^{-1}G)|\psi\rangle$$

$$- \langle\psi|(\mathbb{1}+i r^{-1}G)^{\dagger}H$$

$$\times(\mathbb{1}+i r^{-1}G)|\psi\rangle\Big]$$

$$e^{-i\phi G} = \mathbb{1}\cos(r\phi) -$$

$$i r^{-1} G \sin(r\phi)$$

$$G = \frac{1}{2}\sigma_x, \ \frac{1}{2}\sigma_y \text{ or } \frac{1}{2}\sigma_z$$

$$R = R(\phi) = e^{-i\phi G}$$

$$R\left(\frac{\pi}{2}\right) = \mathbb{1}\cdot\cos\pi/4 - i\,\sigma_x/_2 \sin\pi/4$$

with
$G = \frac{1}{2}\sigma_x$

$$= \frac{1}{\sqrt{2}}\left[\mathbb{1} - i\,\sigma_x\right]$$

$$= \frac{1}{\sqrt{2}}\left(\mathbb{1} - i\,r^{-1}G\right)$$

$$R\left(\frac{\pi}{4\cdot r}\right) = \frac{1}{\sqrt{2}}\left(\mathbb{1} - i\,r^{-1}G\right)$$

$$|\psi\rangle = e^{-i\phi G}|0\rangle$$

$$\frac{\partial\langle H\rangle}{\partial\phi} = \frac{1}{2}\left[\langle H(\phi+\frac{\pi}{2})\rangle - \langle H(\phi-\frac{\pi}{2})\rangle\right]$$

(with $G = \frac{1}{2}\sigma_x, \frac{1}{2}\sigma_y, \frac{1}{2}\sigma_z$)

Gradient descent (GD)

$$\phi^{(j+1)} = \phi^{(j)} - \alpha^{(j)} \frac{\partial \langle H \rangle|_{\phi^{(j)}}}{\partial \phi}$$

- standard GD with a fixed $\alpha^{(j)} = \alpha$ (learning rate)

- GD + momentum

- Stochastic GD
  - Adagrad
  - RMS prop
  - ADAM

$$\left.\begin{matrix} \text{Adagrad} \\ \text{RMS prop} \\ \text{ADAM} \end{matrix}\right\} \alpha^{(j)}$$

$$\alpha^{(j)} \propto \left(\frac{\partial^2 \langle H \rangle}{\partial \phi_j \, \partial \phi_{i}'} \right)^{-1}$$

- quasi-Newton methods
  - Powell
  - Broyden et al.

We have a computational basis $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$\sigma_x |0\rangle = |1\rangle$ (similarly with σ_y)

$$\sigma_z |0\rangle = +1 |0\rangle$$

$$\sigma_z |1\rangle = -1 |1\rangle$$

$|0\rangle$ and $|1\rangle$ are eigenstates of σ_z

$$H \propto \sigma_z w + \sigma_x \gamma$$

$$\sigma_x = \hat{H} \sigma_z \hat{H}$$

$$\sigma_x = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$