WEEK 8 - Giuseppe Carleo

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

Many-body Hamiltonian

Unknown

A) CLASSICALLY (exploit the sparsity) - Week 7

B) QUANTUM COMPUTER - Week 7

$$|\psi(t)\rangle = \hat{U}_p \hat{V}_{p-1} \ldots\ldots \hat{U}_1 |\psi(0)\rangle$$

Trotter Decomposition

⇒ Polynomial Running Time

Ground State Wave Functions

imaginary time

$$|\psi(\tau)\rangle = e^{-\tau\hat{H}}|\psi(0)\rangle$$

$$\lim_{\tau\to\infty} |\psi(\tau)\rangle \simeq |E_0\rangle \quad \text{where} \quad |\langle\psi_0|E_0\rangle| \neq 0$$

Comp. Quant. Phys.

MAJOR <u>OPEN</u> PROBLEM IN CQP IS

HOW TO FIND "GOOD" G.S. WAVE FUNCTIONS

VARIATIONAL METHODS

Variational Principle

$$|\psi(\underbrace{\theta_1 \ldots\ldots \theta_n}_{\text{parameters}})\rangle$$

$$E(\theta_1 \ldots \theta_n) = \frac{\langle \psi(\vec{\theta}) | \hat{H} | \psi(\vec{\theta}) \rangle}{\langle \psi(\vec{\theta}) | \psi(\vec{\theta}) \rangle} \geq E_0$$

$$|\psi(\vec{\theta})\rangle = \sum_k c_k |E_k\rangle \quad \text{where} \quad c_k = \langle E_k | \psi(\vec{\theta}) \rangle$$

$$E(\vec{\theta}) = \sum_{kk'} \frac{\langle E_k | \hat{H} | E_{k'} \rangle \, c_k^* c_{k'}}{\sum_k |c_k|^2}$$

$$= \frac{\sum_k |c_k|^2 E_k}{\sum_k |c_k|^2}$$

γ_k

FIND AN APPROXIMATION FOR THE G.S

Optimization Problem

$$E(\vec{\theta}) \rightsquigarrow \text{Optimal } \theta^* \text{ such that } E(\theta^*) = \text{minimum}$$

$$E(\theta^*) = \arg\min_{\vec{\theta}} E(\vec{\theta}) \geq E_0$$

Compute $E(\theta)$ Classically:

arbitrary operator

$$\frac{\langle\psi|\hat{O}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{k,k'} \langle\psi|k\rangle\langle k|\hat{O}|k'\rangle\langle k'|\psi\rangle}{\sum_k |\langle\psi|k\rangle|^2}$$

$$= \frac{\sum_k |\langle\psi|k\rangle|^2 \sum_{k'} \langle k|\hat{O}|k'\rangle \frac{\langle k'|\psi\rangle}{\langle\psi|k\rangle}}{\sum_k |\langle\psi|k\rangle|^2}$$

$$P(k) = \frac{|\langle\psi|k\rangle|^2}{\sum_{k'} |\langle\psi|k'\rangle|^2} \rightsquigarrow \text{Born's Distribution}$$

$$\langle\hat{O}\rangle = \mathbb{E}_P\left[O_{loc}(k)\right]$$

$\mathbb{E}_P$: statistical expectation value

$O_{loc}(k)$: local operator or estimator

$$O_{loc}(k) = \sum_{k'} \langle k|\hat{O}|k'\rangle \frac{\langle k'|\psi\rangle}{\langle k|\psi\rangle}$$

1) Generate Samples from $P(k)$ (Born Distribution)

$$k_1, k_2, \ldots, k_M \sim P(k)$$

M samples

2) Take the Mean of $O_{loc}(k)$

$$\langle \hat{O} \rangle \simeq \frac{1}{M} \sum_{i=1}^{M} O_{loc}(k_i)$$

$O_{loc}(k)$ is efficient

Generate Samples (with a classical computer)

Markov-Chain Monte Carlo

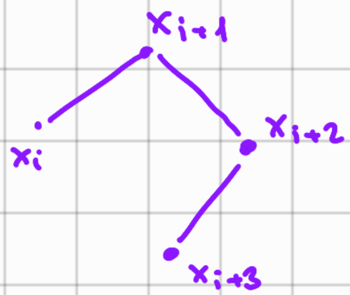
Method to Sample from some $P(k)$

Use a Markov Chain

$$k_1 \to k_2 \to \dots \to k_M$$

$$T(k_i \longrightarrow k_{i+1})$$

Global Transition kernel



Random Walk

(Don't have Memory)

Detailed Balance Condition:

1) $P(k)\, T(k \to k') = P(k')\, T(k' \to k)$

2) If $T(k \to k')$ satisfy 1), then:

$$k_1, k_2, \ldots, k_n \sim P(k)$$

$$T(k_1 \to k_2), \quad T(k_2 \to k_3), \quad \ldots$$

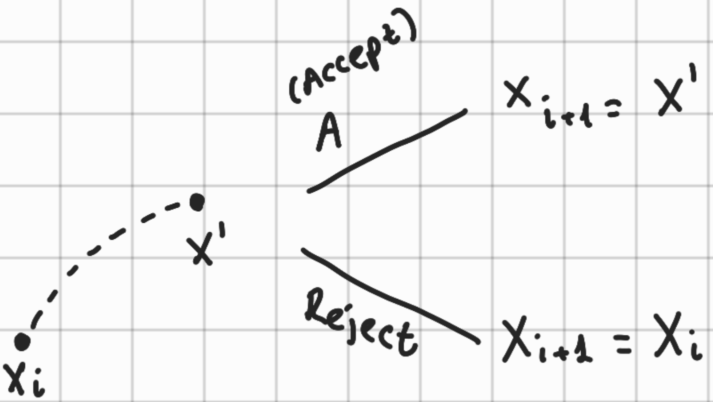
→ Metropolis Algorithm

$$T(k \to k') = T'(k \to k')\, A(k \to k')$$

Global transition kernel (Prob.)

Local Transition kernel (Prob.)

Acceptance kernel (Prob.)



$$A(k \to k') = \min\left(1, \frac{P(k')}{P(k)}\right)$$

if $T'(x \to x') = T'(x' \to x)$

The Algorithm :

1. Generate a random k'

$$T(k_i \longrightarrow k')$$

2. Compute $\frac{P(k')}{P(k_i)} = R$

3. Draw a random uniform number ξ in $(0,1)$

4. $R > \xi$ $\quad k_{i+1} = k'$ ✓ Accept

$R < \xi$ $\quad k_{i+1} = k$ ✗ Reject

Example :

$$\vec{k} = (\sigma_1^z, \sigma_2^z, \ldots, \sigma_N^z)$$

$$= (\pm 1, \pm 1, \ldots, \pm 1)$$

For example, pick 1 spin at random

and then flip it

$$\vec{k} = (+1, \underset{\sim}{-1}, +1)$$

$$\vec{k}' = (+1, +1, +1)$$

$$R = \frac{P(k')}{P(k)} = \frac{|\langle k'|\psi\rangle|^2}{|\langle k|\psi\rangle|^2}$$

This can be computed efficiently if

I have a "black-box" that allows to

compute $\langle k|\psi\rangle = \psi(k;\vec{\theta})$

$\vec{\theta}$ ↘ parameters

Minimize the Energy

$$\langle \hat{H} \rangle = \mathbb{E}_p\left[E_{loc}(k)\right] = E(\vec{\theta})$$

$$E_{loc}(k) = \sum_{k'} \langle k|\hat{H}|k'\rangle \frac{\langle k'|\psi\rangle}{\langle k|\psi\rangle}$$

If $|\psi(\vec{\theta})\rangle$

$$\frac{\partial}{\partial\theta_\ell} E(\vec{\theta}) = \mathbb{E}_p\left[E_{loc}(k)\, D_\ell^*(k)\right] +$$

$$- \mathbb{E}_p\left[E_{loc}(k)\right] \mathbb{E}_p\left[D_\ell^*(k)\right] + c.c$$

complex ? conj

$$D_\ell(k) = \left[\frac{\partial}{\partial\theta_\ell}\langle k|\psi(\vec{\theta})\rangle\right] \frac{1}{\langle k|\psi\rangle} = \frac{\partial}{\partial\theta_\ell} \log \langle k|\psi(\vec{\theta})\rangle$$

Variational Monte Carlo

0) Random Parameters $\vec{\theta}^{(0)}$

1) $P(k_i, \vec{\theta}^{(i)}) \longrightarrow \vec{k_1}, \dots, \vec{k_m}$

(sort of iterative loop)

2) Estimate $E(\vec{\theta}^{(i)})$, $\frac{\partial}{\partial \theta_l} E(\vec{\theta}^{(i)})$

3) $\vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \frac{\partial}{\partial \theta_l} E(\vec{\theta}^{(i)})$ Update parameters

$\searrow$ Similar to Machine Learning

4) Repeat I - III

Example Black Boxes

I Mean Field Black Box

$$\langle \sigma_1^z, \dots, \sigma_N^z \mid \Psi(\vec{\theta}) \rangle =$$

$$= \langle \sigma_1^z \dots \sigma_N^z \mid [\,|\phi_1\rangle \otimes |\phi_2\rangle \dots \otimes |\phi_N\rangle\,]$$

$$= \langle \sigma_1^z | \phi_1 \rangle \langle \sigma_2^z | \phi_2^z \rangle \dots\dots \langle \sigma_N^z | \phi_N^z \rangle$$

$\downarrow$

Variational Parameters are Single-Spin Amplitudes

$$\theta_1 = \langle \uparrow | \phi_1 \rangle$$

$$\theta_2 = \langle \downarrow | \phi_2 \rangle$$

$$\vdots$$

II Neural Quantum States

Deep Networks

Black Box

$$\langle k | \Psi(\vec{\theta}) \rangle = F(\vec{k}, \vec{\theta})$$

$\searrow$ neural network

VARIATIONAL QUANTUM ALGORITHMS

Parameterized Ansatz

$\downarrow$

is a quantum circuit

$$\hat{U}(\vec{\vartheta}) = \hat{U}_\ell(\vartheta_\ell)\, \hat{U}_{\ell-1}(\vartheta_{\ell-1}) \;\ldots\ldots\; \hat{U}_1(\vartheta_1)$$

variational param.

Exp $\quad \hat{U}_1(\vartheta_1) = \exp\left[-i\,\frac{\theta_1}{2}\,\hat{X}_1\right]$

(I) $|\psi(\vec{\vartheta})\rangle = \hat{U}(\vec{\vartheta})\,|0\rangle$

(II) $E(\vec{\vartheta}) = \langle \psi(\vec{\vartheta})|\,\hat{H}\,|\psi(\vec{\vartheta})\rangle$

(III) $\dfrac{\partial E(\vec{\vartheta})}{\partial \vartheta_\ell} = G_\ell(\vec{\vartheta})$

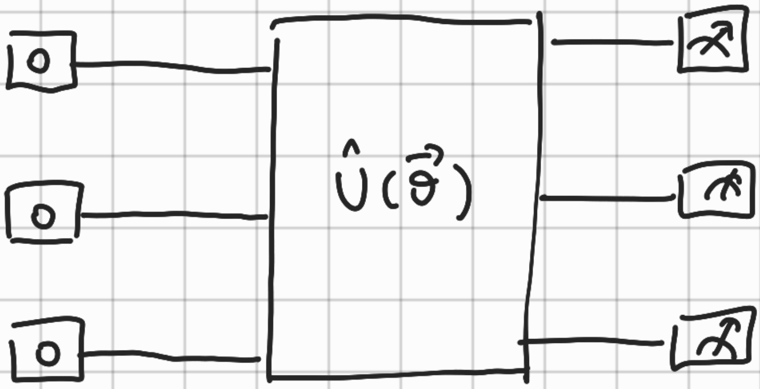
(IV) $\vec{\vartheta}^{(i+1)} = \vec{\vartheta}^{(i)} - q\,\vec{G}^{(i)}$

Expected Value of the Energy

$$\hat{H} = -\Gamma \sum_i \hat{X}_i + \sum_i J\, \hat{Z}_i\, \hat{Z}_{i+1}$$

Diagonal term:

$$\langle \psi(\vec{\vartheta})\,|\,\hat{Z}_i\,\hat{Z}_{i+1}\,|\,\psi(\vec{\vartheta})\rangle$$



$$P(z_1, z_2, z_3) = |\langle z_1 z_2 z_3 | \psi \rangle|^2$$

$$\langle z_1 z_2 \rangle = \frac{1}{M} \sum_{i=1}^{M} z_1^{(i)} z_2^{(i)}$$

$$\langle \psi | z_1 z_2 | \psi \rangle = \sum_{\vec{z}, \vec{z}'} \langle \psi | \vec{z} \rangle \langle \vec{z} | \hat{z}_1 \hat{z}_2 | \vec{z}' \rangle \langle \vec{z}' | \psi \rangle$$

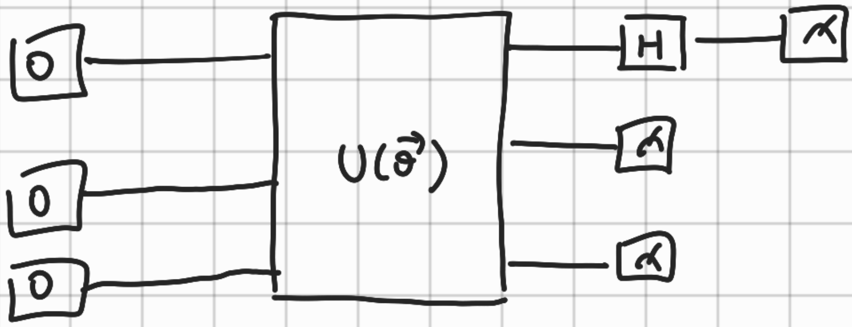
$(\vec{z} = (z_1, z_2, \dots z_n))$

observable

$$= \sum_{\vec{z}} |\langle \psi | z \rangle|^2 \; z_1 z_2 \qquad \simeq E_{p(\vec{z})} [z_1 z_2]$$

Estimate $\hat{X}_i$

$$\langle \psi | \hat{X}_1 | \psi \rangle = \langle \psi | \hat{H}_1 \hat{Z}_1 \hat{H}_1 | \psi \rangle$$



$z_1 = \pm 1$

$$\langle \hat{X}_1 \rangle = \frac{1}{M} \sum_i z_1^{(i)}$$

$$\langle \hat{X}_2 \rangle = \frac{1}{M} \sum_i z_2^{(i)}$$

(III) Computing the gradients of the Energy

$$\hat{U}_k(\theta_k) = \exp\left[-i \frac{\theta_k}{2} \underbrace{\hat{S}_k}_{\text{some operator}} \right]$$

e.g. $\hat{S}_k = (\hat{x}, \hat{y}, \hat{z}) \rightarrow$ single qubit operations

or $\hat{S}_k = (\hat{x}\hat{x}, \hat{z}\hat{z}, \ldots) \rightarrow$ two qubit opr.

$\hat{S}_k$ is a product of Pauli matrices

$\hat{S}_k^2 = \mathbb{I}$, involutory

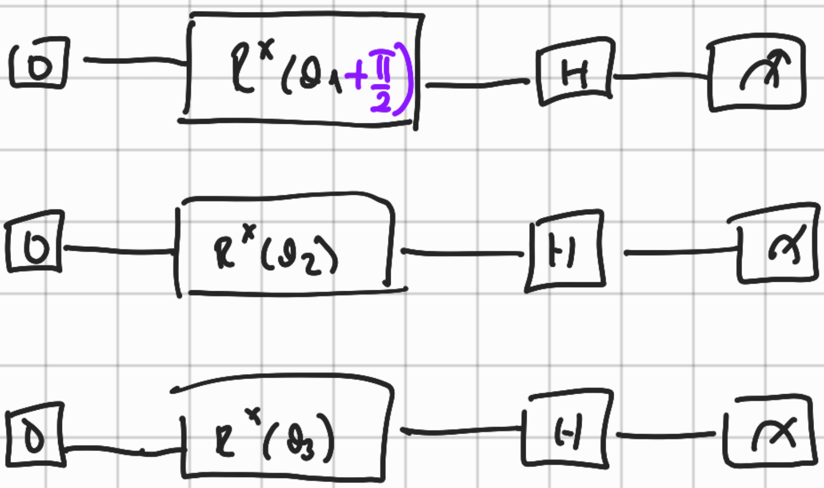
Parameter - Shift Rule

$$\frac{\partial E}{\partial \theta_\ell} = \frac{E(\theta_1, \dots \theta_\ell + \frac{\pi}{2}, \dots \theta_N) - E(\theta_1, \dots \theta_\ell - \frac{\pi}{2}, \dots \theta_N)}{2}$$

Example: $|\psi(\theta)\rangle = R_3^x(\theta_3)\, R_2^x(\theta_2)\, R_1^x(\theta_1)\, |0\rangle$

$$\hat{H} = \hat{X}_1 + \hat{X}_2 + \hat{X}_3$$

Hamiltonian



$\rightarrow E(\theta_1 + \frac{\pi}{2}, \theta_2, \theta_3)$

Adiabatic State Preparation

$$\hat{H}(t) = \left(1 - \frac{t}{t_f}\right)\hat{H}_0 + \frac{t}{t_f}\hat{H}_f$$

$\hat{H}_0$: driving hamiltonian

$\hat{H}_f$: target hamiltonian

$t_f > 0$ fixed at the beginning of the simulation

$$|\Psi(0)\rangle \longrightarrow |\Psi(t_f)\rangle$$

$$H(t), \quad |\Psi(t_f)\rangle \neq e^{-iH(t)t_f}|\Psi(0)\rangle$$

$$H(0) = \hat{H}_0, \qquad H(t_f) = \hat{H}_f$$

Adiabatic Theorem

If $t_f \gg \min_t \left(\frac{1}{\Delta(t)^2}\right) \rightsquigarrow |\Psi(t)\rangle$ is in the ground state of $\hat{H}(t)$

$\Delta t = E_1^t - E_0^t$ (instantaneous gap)

$|\Psi(0)\rangle = |E_0^0\rangle$

$|\Psi(t)\rangle = |E_0^t\rangle$

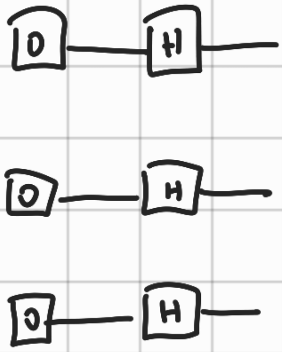
$|\Psi(t_f)\rangle = |E_0^{t_f}\rangle$

$$|E_0^t\rangle \longrightarrow \hat{H}(t)|E_0^t\rangle = \mathcal{E}_0^t\,|E_0^t\rangle$$

with $\mathcal{E}_0^t \le \mathcal{E}_1^t$ .....

<u>Ex:</u> TF Ising Model

$$\hat{H}_0 = -\Gamma\sum_i X_i\,, \qquad |\psi(0)\rangle =$$

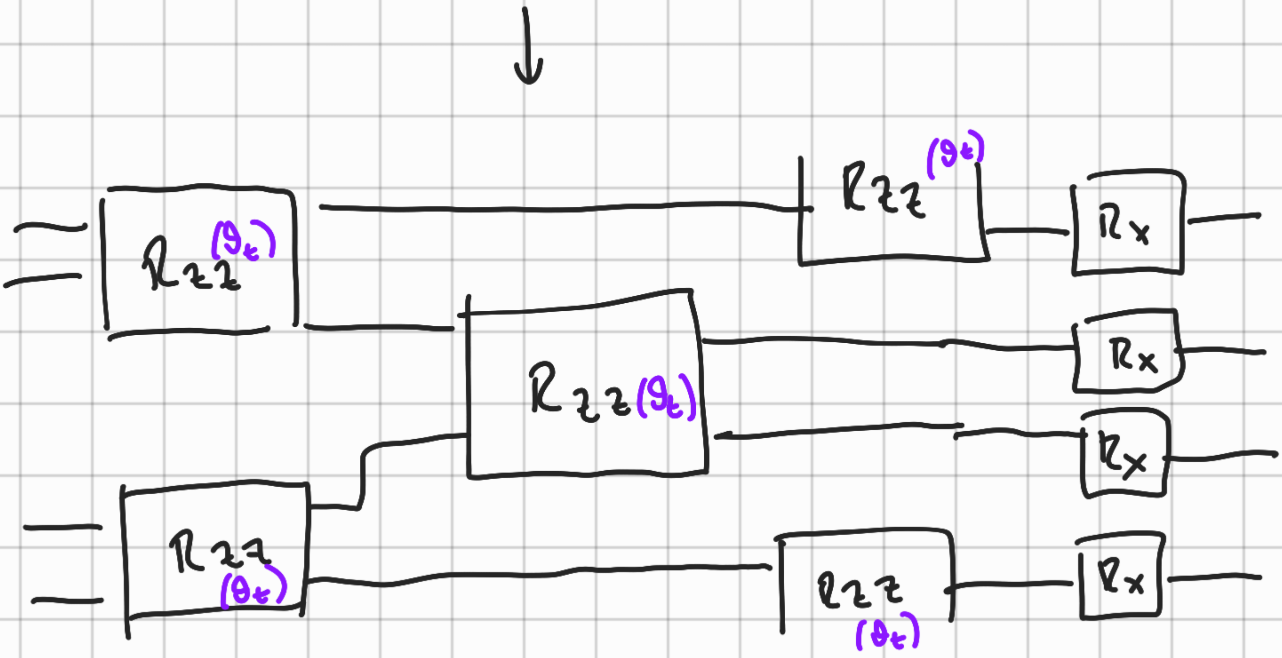


$$\hat{H}(t) = -\Gamma\left(1-\frac{t}{t_f}\right)\sum_i X_i - \left(\frac{t}{t_f}\right)\Gamma\sum_i X_i + \frac{t}{t_f}J\sum_i \hat{Z}_i\hat{Z}_{i+1}$$

$$= -\Gamma\sum_i \hat{X}_i + \frac{t}{t_f}J\sum_i \hat{Z}_i\hat{Z}_{i+1}$$

$$|\psi(t+\delta_t)\rangle = e^{-i\hat{H}(t)\delta_t}\,|\psi(t)\rangle$$

Trotterization



$$\exp\left[-i\,\delta_t\, z_i\, z_{i+1}\right] \qquad \exp\left[-i\,\delta_t\, X_i\right]$$

$$\theta_t = \delta_t \frac{t}{t_f} J$$