بسم الله الرحمن الرحیم ۱۴۰۰/۹/۲۱ جبر

* Variational Monte Carlo

① The $\underbrace{\text{Variational Principle}}_{\text{اصل وردش}}$ provide a robust method to find a ground state of typical $\underbrace{\text{many-Body}}_{\text{بس ذره ای}}$ system

② Consider a typical $\overbrace{\text{Many-Particle}}^{\text{N-Particle}}$ Hamiltonian as below:

$$\mathcal{H} = \mathcal{H}_{Kinetic} + U \longrightarrow \{\text{Intraction}\}$$

$\mathcal{H}_{Kinetic} \longrightarrow$ Kinetic Part

$$\mathcal{H}_{Kinetic} = \sum_{i=1}^{N} \frac{|\vec{P}_i|^2}{2m} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} |\vec{\nabla}_i|^2$$

$$U = \sum_{i=0}^{N} U_{ext}(\vec{r}_i) + \sum_{i,j=1}^{N}{}' U_{int}(r_{ij})$$

$\sum'$: $i \neq j$; $i < j$

$U_{int}(r_{ij}) \longrightarrow$ Pairwise

Fermion $\boxed{\text{Anti-Symmetric}}$

Well-Symmetric wavefunction

$\boxed{\text{Boson fully Symmetric}}$

{ Chapter 10, 11, 12 of Pathria }

③ $$\boxed{\mathcal{H}\varphi_n = E_n \varphi_n}$$

φ_n is the nth of eigenwavefunction

E_n is eigenvalue

$\varphi_n = ?$, $E_n = ?$ $\longrightarrow$ $\left\{ \begin{array}{l} E_0 \text{ \&} \\ \varphi_0 \end{array} \right\}$ ground state

④ The Purpose of variational approach is to find a <u>wave function</u> that can be optimized to produce a closest expectation value of $\langle \mathcal{H} \rangle$ to the ground state

Energy

$$\langle \mathcal{H} \rangle_\psi = E \longrightarrow E_0$$

a typical Wavefunction

We are interested in finding a method to map the <u>eigenvalue Problem</u> to <u>importance Sampling approach</u>

E_0

$\boxed{\text{Variational MC}}$

(5) Example : Time-Independent Schrodinger Equation

Quantum Harmonic oscillator in 1D

$$\begin{cases} \hat{H}\psi = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right] \psi \\ \underline{\underline{\mathcal{H}}}\psi = E\psi \end{cases}$$

$H_0(x) = 1, \; H_1(x) = 2x \ldots$

Hermite polynomial

ویژه مقدار $\rightarrow$ $E_n = (n + \frac{1}{2})\hbar\omega$

ویژه تابع $\rightarrow$ $$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) e^{-\frac{m\omega x^2}{2\hbar}}}$$

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(6) Variational Principle

$$\mathcal{H}\varphi_n(x) = E_n \varphi_n(x)$$

$\begin{cases} E_n = \text{eigenvalue} \\ \varphi_n = \text{eigenfunction} \end{cases}$

$$\underline{\mathcal{H}}\varphi_0(x) = E_0 \underline{\varphi_0(x)}$$

$\begin{cases} E_0 = ? \\ \varphi_0 = ? \end{cases}$

$\underbrace{\psi(x)}$: a typical arbitrary wave function

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$$\langle \mathcal{H} \rangle_\psi = E$$

bases func

$$\psi(x) = \sum_n C_n \varphi_n$$

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$$E = \langle \mathcal{H} \rangle_\psi = \frac{\langle \psi | \mathcal{H} | \psi \rangle}{\langle \psi | \psi \rangle}$$

$$E = \text{''} = \frac{\int dx\, \psi^*(x)\, \mathcal{H}\, \psi(x)}{\int dx\, \psi^*(x)\, \psi(x)}$$

In principle this value can be as close as we want to E_0 of $\mathcal{H}$

$$\boxed{E \longrightarrow E_0}$$

$$\left\{ \begin{array}{l} E = \langle \mathcal{H} \rangle_\psi \geqslant E_0 \quad \text{for any arbitrary } \psi \\ \text{and } \boxed{E = E_0} \text{ if and only if } \psi = C_0 \varphi_0 \end{array} \right\}$$

$$\mathcal{H}\varphi_n(x) = E_n\varphi_n(x) \qquad \int \varphi_n^*(x)\,\varphi_m(x)\,dx = \delta_{nm}$$

باید تابع موج دلخواه

$$\psi(x) = \sum_n C_n \varphi_n(x)$$

$$E = \langle \mathcal{H} \rangle_\psi = \frac{\int dx\, \psi^*(x)\, \mathcal{H}\psi(x)}{\int dx\, \psi^*(x)\,\psi(x)}$$

$$E = \frac{\sum_{nm} C_n^* E_n C_m \int dx\, \varphi_n^*(x)\,\varphi_m(x)}{\sum_{nm} C_n^* C_m \underbrace{\int dx\, \varphi_n^*(x)\,\varphi_m(x)}}$$

$$E = \frac{\sum_{n=0}^{\infty} |C_n|^2 E_n}{\sum_{n=0}^{\infty} |C_n|^2} = E_0 + \frac{\sum_{n=1}^{\infty} |C_n|^2 E_n}{\sum_{n=0}^{\infty} |C_n|^2}$$

$$E = E_0 + \frac{\sum_{n=0}^{\infty} |C_n|^2 (E_n - E_0)}{\underbrace{\sum_{n=0}^{\infty} |C_n|^2}}$$

$E_n \geq E_0$

$n = 0, 1, 2 \ldots$

$$\underbrace{E = E_0 + \overbrace{\cdots\cdots\cdots}^{\text{positive definit}}}$$

$$\boxed{E \geqslant E_0}$$

The minimum value of our Estimated "E" is an upper limit of ground State.

(7) $$\psi(x;\{\theta\}) \longrightarrow \underline{\psi(x;\{\theta\}_{Best})}$$

trial wave funct

$$\mathrm{Min}\{E\} \simeq E_0$$

$$E \geqslant E_0$$

$$\boxed{\text{Variational MC}}$$

(8) Variational MC

(A) $$\psi_T(\{\theta\}, x) = $$

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$$\{\theta\}_d : \overbrace{\{\theta_1, \theta_2 \ldots \theta_M\}}$$

(B) $$E(\{\theta\}) = \langle \mathcal{H} \rangle_{\psi_T} = \frac{\int dx\, \psi_T^*(\{\theta\},x)\, \mathcal{H}\, \psi_T(\{\theta\},x)}{\int dx\, \psi_T^*(\{\theta\},x)\, \psi_T(\{\theta\},x)}$$

$\{x\} \equiv \{\bar{r}_1, \bar{r}_2 \ldots \bar{r}_N\}$. $N \equiv$ # of particles in system

(C) $$P(\{\theta\},x) \equiv \frac{|\psi_T(\{\theta\},x)|^2}{\int dx\, |\psi_T(\{\theta\},x)|^2}$$

(D) (B) and (C) $\rightarrow$

$$E(\{\theta\}) = \frac{\int dx\, \psi_T^*(\{\theta\},x)\, \frac{\psi_T(\{\theta\},x)}{\psi_T(\{\theta\},x)}\, \mathcal{H}\, \psi_T(\{\theta\},x)}{\int dx\, |\psi_T(\{\theta\},x)|^2}$$

$|\psi_T(\{\theta\},x)|^2$

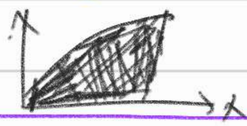
$$= \frac{\int dx\, |\psi_T(\{\theta\},x)|^2\, \frac{\mathcal{H}\psi_T(\{\theta\},x)}{\psi_T(\{\theta\},x)}}{\int dx\, |\psi_T(\{\theta\},x)|^2}$$

$$E(\{\theta\}) = \int dx\; P(\{\theta\},x)\, \frac{\mathcal{H}\psi_T(\{\theta\},x)}{\psi_T(\{\theta\},x)}$$

$$E(\{\theta\}) = \int dx \; p(\{\theta\}, x) \; E_L(\{\theta\}, x)$$

$\int dx \, A(x)$

probability



Recall $\langle f \rangle = \int dx \; f \, \rho(x) = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$

X_i can be generat with probabilt $\rho(x)$

$$E(\{\theta\}) = \frac{1}{N} \sum_{i=1}^{N} E_L(\{\theta\}, X_i) \, p(\{\theta\}, x_i)$$

X_i با احتمال p تولید شده سپس وزن دهی می‌شوند.

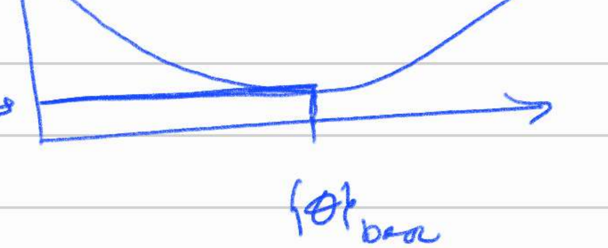
$$E(\{\theta\}) = \frac{1}{N} \sum_{i=1}^{N} E_L(\{\theta\}, X_i)$$

$p(\{\theta\}, X)$

for a given set of $\{\theta\}$.

$E(\{\theta\})$

$\tilde{E}_0 \geqslant E_0$



* for a given set of $\{\theta\}$. *

we should produce $\{X\}$ with

probability given by $P(\{\theta\}, X)$

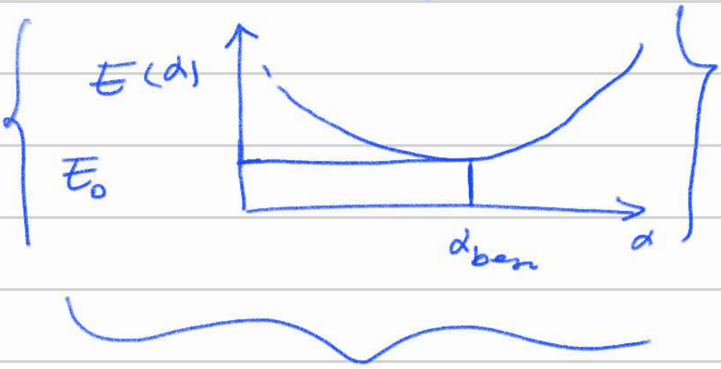
* and compute $E(\{\theta\})$ *

Ex 2 $\quad \mathcal{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 \qquad \left\{ \begin{array}{l} m=1 \\ \hbar=1 \\ \omega=1 \end{array} \right\}$

$$\left\{ \begin{array}{l} \varphi_0 = ? \\ E_0 = ? \end{array} \right.$$

we choose the following trial wave function to solve our problem

$$\psi_T(\theta, x) = e^{-\alpha x^2} \qquad \alpha = ?$$



$$E(\alpha) = \int dx \; p(\alpha, x) \; E_L(\alpha, x)$$

$$E_L(\alpha, x) = \frac{\mathcal{H}\,\psi_T(\alpha, x)}{\psi_T(\alpha, x)} = \frac{\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2\right) e^{-\alpha x^2}}{e^{-\alpha x^2}}$$

$$\boxed{E_L(\alpha, x) = \alpha + x^2\left(\frac{1}{2} - 2x^2\right)}$$

$$p(\alpha, x) = \frac{|\psi_T(\alpha, x)|^2}{\int dx\, |\psi_T(\alpha, x)|^2} \sim e^{-2\alpha x^2}$$

$$\{x_1, x_2, \ldots, x_N\}$$

$$E(\alpha) = \frac{1}{N} \sum_{i=1}^{N} \left[\alpha + x_i^2\left(\frac{1}{2} - 2x_i^2\right)\right]$$

این سری که هر x تولید می‌شود لازم است از این تابع $p(\alpha, x) = e^{-2\alpha x^2}$ پیروی کند.

Loop $\boxed{\alpha = \alpha_{min}, \; \alpha_{max}}$

Metropolis-step

loop $i = 1, N$

Select x_i according to $p(\alpha, x_i)$

$E(\alpha) = E(\alpha) + E_L(\alpha, x_i)$

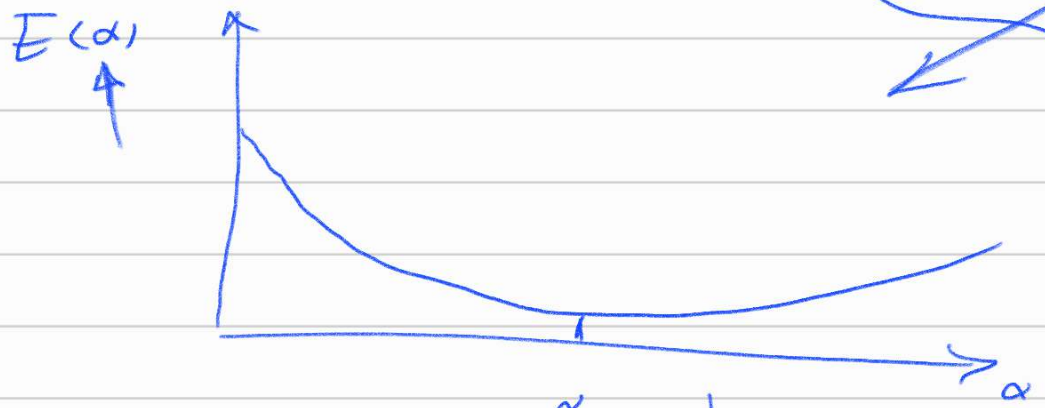
End loop

$$E(\alpha) = \frac{E(\alpha)}{N}$$

Write α . $E(\alpha)$

End loop

A typical VMC algorithm



$\alpha_{best} = 1/2 \longrightarrow$ Analytical Soln

$$\boxed{\text{Importance Sampling + Metropolis + MCMC (HMC)}}$$

$\{X\}, \{\theta\}$