Variational Monte carlo method

Eigen Vector
Dizen Value
of a given Hamilton:

Ex Quantum harmonic oscillator in 10

$$
\eta t \psi(x)=\left[-\frac{\hbar^{2}}{2 m} \frac{d^{2}}{d x^{2}}+\frac{1}{2} m \omega^{2} x^{2}\right] \psi(x)
$$

$$
=E f(x)
$$



$$
\left\{\begin{array}{l}
E_{n}=(n+1 / 2) \hbar \omega \\
\Psi_{n}(x)=\left(\frac{m \omega}{\pi \hbar}\right)^{1 / 4} \frac{1}{\sqrt{2^{n} n!}} \\
H_{n}\left(x \sqrt{\frac{m \omega}{\hbar}}\right) e^{\sim^{-\frac{m \omega x^{2}}{2 \hbar}}} \\
\underset{\text { Hermit te polynomial }}{H_{0}(x)=1,} \quad H_{1}(x)=2 x, \quad H_{2}(x)=2\left(x^{2}-2\right.
\end{array}\right.
$$


r!
Variational Theorem -

Recall: Variational theorem
MC: ©


$$
\downarrow
$$ Z E.

$$
\left\{\begin{array}{r}
\vec{E}=\langle\mathcal{H}\rangle_{\psi} \geqslant E_{0} \quad \text { for any arbitrary } \psi \\
\text { and } E=E_{0} \quad \text { if and only if } \\
\mu(x)=C . \varphi_{0}(x)
\end{array}\right\}
$$

$$
\begin{aligned}
& H \varphi_{n}(x)=E_{n} \varphi_{n}(x) \\
& \text { 20 } \\
& \mathcal{H} \varphi_{0}(x)=\stackrel{\downarrow}{E_{0}} \varphi_{0}(x) \\
& 0, x, c=2(x)=\sum_{n} C_{n} \varphi_{n}(x) \\
& E=\langle\mathcal{H}\rangle=\frac{\langle\psi(x)| \mathcal{H}|\psi(x)\rangle}{\langle\psi(x) \mid \psi(x)\rangle} \\
& E=\frac{\int d x \psi^{*}(x) \notin \psi(x)}{\int d x \psi^{*}(x) \psi(x)}
\end{aligned}
$$

$$
\begin{aligned}
& \mathcal{H} \varphi_{n}(x)=E_{n} \varphi_{n}(x) \\
& \int d x \varphi_{n}^{*}(x) \varphi_{m}(x)=\delta_{n m} \\
& E=\langle\eta\rangle=\frac{\int d x \psi^{*}(x) H(x)=\sum_{n} C_{n} \varphi_{n}(x)}{\int d x \psi_{(x)}^{*}(x) \psi(x)} \\
& E=\frac{\sum_{n m} C_{n}^{*} E_{n} C_{n} \int d x \varphi_{n}^{*}(x) \varphi_{m}(x)}{\sum_{n m} C_{n}^{*} C_{m} \int d x \varphi_{n}^{*}(x) \varphi_{m}(x)} \\
& E=\frac{\sum_{n=0}^{\infty}\left|C_{n}\right|^{2} E_{n}}{\sum_{n=0}^{\infty}\left|C_{n}\right|^{2}}=E_{0}+\frac{\sum_{n=0}^{\infty}\left|C_{n}\right|^{2}\left(E_{n}-E_{0}\right)}{\sum_{n=0}^{\infty}\left|C_{n}\right|^{2}} \\
& E=E \cdot 0 \\
& E_{0}+E_{0} n n=0,1, \ldots \\
& \cdots \frac{E_{n}}{\mid E \geqslant E_{0}}
\end{aligned}
$$

Variational MC
 U

$$
\underset{\uparrow}{E(\{\alpha\}} \underset{\substack{\{1 \\ \text { Best }}}{ }\}) \rightarrow E_{0}(\mathcal{H}:=\infty)
$$


$E \geqslant E_{0}=$ Energy of Ground Stake
(1) $\psi_{T}(\{\alpha\}, x),\{\alpha\}:\left\{\alpha_{1} \ldots \alpha_{s}\right\}$ Free parameters
(2)

$$
\begin{array}{r}
E(\{\alpha\})=\langle\mathcal{H}\rangle_{\tau}=\frac{\int d x \psi_{T}^{*}(\{\alpha\}, x) \mathcal{H} \psi_{T}(\{d\}, x)}{\int d x \psi_{T}^{*}(\{\alpha\}, x) \psi_{T}(\{\alpha\}, x)} \\
x \equiv\left\{r_{1}, r_{2}, \ldots r_{N}\right\} \quad N=\text { of Particles } \\
\text { Many Body }
\end{array}
$$

$$
\begin{aligned}
& \text { (3) } \underset{\substack{p(\{\alpha\}, x)}}{\left.\int d \dot{\omega}\right)}=\frac{\left|\psi_{T}(\{\alpha\}, x)\right|^{2}}{\int d x\left|\psi_{T}(\{\alpha\}, x)\right|^{2}}\left|\psi_{T}(\{\alpha\}, x)\right|^{2} \\
& E(\{\alpha\})=\frac{\int d x \frac{\tilde{\psi}_{T}^{*}(\{\alpha\}, x) \psi_{T}(\{\alpha\}, x)}{\left.\psi_{T}\{\alpha\}, x\right)}}{\int t \psi_{T}(\{\alpha\}, x)} \underset{\int d x\left|\psi_{T}(\{\alpha\}, x)\right|^{2}}{ } \\
& E(\{\alpha\})=\frac{\int d x \int \frac{\mid \psi_{T}\left(\left.\{\alpha,, x)\right|^{2}\right.}{\iint d x\left|\psi_{T}(\{\alpha\}, x)\right|^{2}} \frac{\psi_{T}(\{\alpha\}, x)}{\psi_{T}(\{\alpha\}, x)}}{\int} \\
& E(\{\alpha\})=\int d x \quad P(\{\alpha\}, x)\left(\frac{\mathcal{H}_{T}(\{\alpha\}, x)}{\psi(\{\alpha\}, x)}\right)
\end{aligned}
$$

$$
=\int d x p(\{\alpha\}, x) \frac{\downarrow}{E_{L}}(\{\alpha\}, x)
$$

$\downarrow$
beal Energy


$$
\left\{\langle f\rangle=\int d x f(\underset{\sim}{\sqrt{1}}(x)\}\right.
$$





$$
E(\{\alpha\})=\frac{1}{M} \sum_{i=1}^{M} E_{L}\left(\{\alpha\}, x_{i}\right) P\left(\{\alpha\}, x_{i}\right)
$$





巨ín

$$
\begin{aligned}
& E(\{\alpha\}) \underbrace{\longrightarrow}_{\swarrow \quad\{\alpha\}} \\
& \{\alpha\}=\left\{\alpha_{\text {Best }}\right\} \longrightarrow \quad E \sim E_{0} \\
& \text { كَحْ } \\
& E_{x}: \rightarrow t=-1 / 2 \frac{d^{2}}{d x^{2}}+\frac{1}{2} x^{2} \\
& m=1 \\
& \hbar=1 \\
& \omega \rightarrow 1 \\
& \rightarrow \psi_{T}(\{\alpha\}, x)=e^{-\alpha x^{2}} \\
& \text { زنه }
\end{aligned}
$$

$$
\begin{aligned}
& E(\alpha)=\frac{1}{M} \sum_{i=1}^{M} E_{L}\left(\alpha, x_{i}\right) \\
& \text { 多 } \\
& E_{L}(\alpha, x)=\frac{\eta t \psi_{T}(\alpha, x)}{\psi_{T}(\alpha, x)}=\frac{\left(-\frac{1}{2} \frac{d^{2}}{d x^{2}}+\frac{1}{2} x^{2}\right) e^{-\alpha x^{2}}}{e^{-\alpha x^{2}}} \\
& \text { * } E_{L}(\alpha, x)=\alpha+x^{2}\left(\frac{1}{2}-2 \alpha^{2}\right) \\
& \rightarrow P(\alpha, x)=\frac{\left|\psi_{T}(\alpha, x)\right|^{2}}{\int d x\left|\psi_{T}(\alpha, x)\right|^{2}} \sim e^{-2 \alpha x^{2}} \\
& T \rightarrow 1 \sum_{\left.\alpha+x^{2} \cdot\left(1-2 \alpha^{2}\right)\right\rceil}
\end{aligned}
$$

$$
t(a)=\bar{M}<_{i=1} l^{\cdots} \cdot \bar{L}^{-}
$$



$$
\begin{aligned}
& {\left[\text { loop } \quad \alpha=\alpha_{\text {min }}, \alpha_{\text {max }}, \Delta \alpha\right.}
\end{aligned}
$$

$$
\begin{aligned}
& E(\alpha)=\frac{E(\alpha)}{M}
\end{aligned}
$$

Write $\alpha$, $E(\alpha)$

$$
\rightarrow \text { End loop }
$$

for $E_{m, i}(\alpha)=E\left(\alpha, \alpha_{\text {Best }}\right)$
-

$$
\left\{\alpha_{1}(\text { Best }), \alpha_{2}(\text { Best }), \alpha_{3}(\text { Best }), \alpha_{4}\{\text { Best }), \alpha_{5}(\text { Best })\right\}
$$


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