FYS 4411/9411, JANUARY 26, 2023

VMC - basics

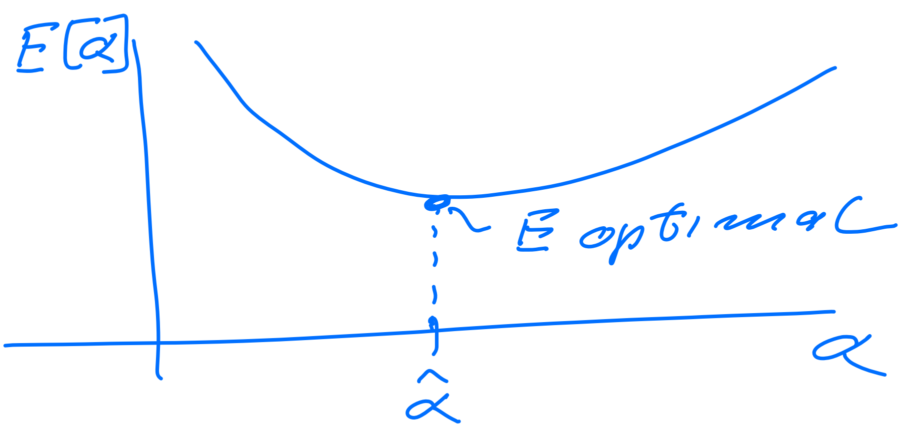
- Define trial wave function

$$\psi_T(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \sigma_1, \sigma_2, \ldots \sigma_N; \vec{\alpha})$$

$\vec{\alpha} = \{\alpha_1, \alpha_2, \ldots, \alpha_m\}$
variational parameters

$$E[\hat{\vec{\alpha}}] = \underset{\alpha \in \mathbb{R}^m}{\operatorname{argmin}} \frac{\int d\vec{r}_1 d\vec{r}_2 \ldots \times \psi_T^*(\vec{r}_1, \ldots) \hat{H} \psi_T(\vec{r}_1, \ldots)}{\int d\vec{r}_1 \ldots d\vec{r}_N |\psi_T|^2}$$

Vary $\vec{\alpha}$ in order to find the minimal energy.



Convex optimization problem.

Standard definition of an expectation value

$$\mathbb{E}[x] = \int_{x \in D} dx\, x\, p(x)$$

$$\int_{x \in D} dx\, p(x) = 1$$

Rewrite $E[\alpha]$

Define the probability

$$p(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N; \sigma_1, \sigma_2 \dots \sigma_N; \vec{\alpha})$$

$$= p(\vec{R}; \vec{\alpha})$$

$$\vec{R} = (\vec{r}_1, \vec{r}_2, \dots \vec{r}_N; \sigma_1, \sigma_2 \dots \sigma_N)$$

$$p(\vec{R}; \vec{\alpha}) = \frac{|\Psi_T(\vec{R}; \vec{\alpha})|^2}{\int d\vec{R}\, |\Psi_T(\vec{R}; \vec{\alpha})|^2}$$

Define local energy

$$E_L(\vec{R};\vec{\alpha}) = \frac{1}{\psi_T(\vec{R};\vec{\alpha})} H(\vec{R})\,\psi_T(\vec{R};\vec{\alpha})$$

$$E[\vec{\alpha}] = \frac{\int d\vec{R}\, \psi_T^* H \psi_T}{\int d\vec{R}\, |\psi_T|^2}$$

$$= \int P(\vec{R};\vec{\alpha})\, E_L(\vec{R};\vec{\alpha})\, d\vec{R}$$

$$\simeq \frac{1}{MCS} \sum_{i=1}^{MCS} E_L(\vec{R}_i;\vec{\alpha})$$

MCS = # MonteCarlo samples

Basics of algorithm

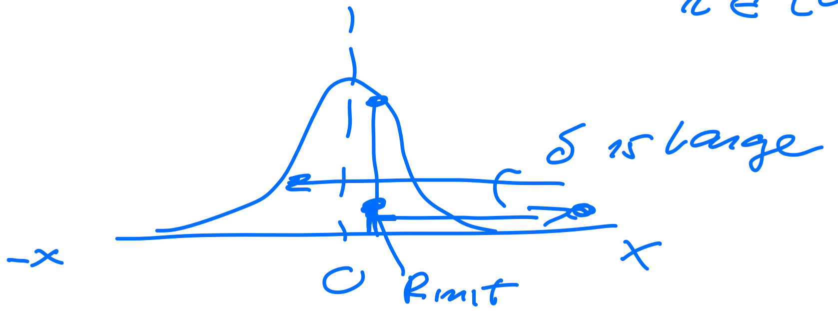
initialize

- Define # MCS
- Define initial position $\vec{R}_{init}$
- Define $\vec{\alpha} = \{\alpha_1, \alpha_2 \ldots \alpha_M\}$
- Define $E[\alpha] = 0$
- Define $\delta\, \mathrm{var}(E[\alpha])$

For $i = 1, MCS$

- calculate a new trial $\vec{R} = \vec{R}_{init} + r \cdot \delta$

$r \in [0,1]$ step size



- Metropolis's algorithm

accept if $w = \frac{P(\vec{R})}{P(\vec{R}_{init})} \le r'$

$r' \in [0,1]$

- if step accepted

$\vec{R}_{new} = \vec{R} = \vec{R}_{init} + r \cdot \delta$

- update averages

End For loop.

<u>Example</u> : harmonic oscillator

$\hbar = c = m = 1 = \omega$

$\psi_T(x;\alpha) = \exp\left(-\frac{1}{2}\alpha^2 x^2\right)$

$E_L[x;\alpha] = \frac{1}{\psi_T}\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2\right]\psi_T$

$$= \frac{1}{2}\left(\alpha^2 + x^2\left(1-\alpha^4\right)\right)$$

$$E[\alpha] = \int_{-\infty}^{\infty} P(x;\alpha)\, E_L[x;\alpha]\, dx$$

$$= \frac{1}{4}\left(\alpha^2 + \frac{1}{\alpha^2}\right)$$

Find α-optimal

$$\frac{dE[\alpha]}{d\alpha} = 0 \quad \Rightarrow$$

$$\alpha = 1$$

$$var[E[\alpha]] = \mathbb{E}\left[\int E_L^2 p\, dx - E^2[\alpha]\right]$$

$$= \frac{1}{4}\left(1 + \left(1-\alpha^4\right)^2 \frac{3}{4\alpha^4}\right)$$

$$- \left(E[\alpha]\right)^2$$