FYS4411/9411 Lecture Feb 11

Towards the Fokker-Planck eq:

– 1st digression

$$P_i^{(t+\Delta t)} \rightarrow \underline{P(\vec{y}, t+\Delta t)}$$

$$= \int W(\underline{\vec{y}, t+\Delta t | \vec{x}, t}) P(\vec{x}, t) d\vec{x}$$

Markov chain

How do we translate this into quantum mech?

$$\hat{H}|\Phi_0\rangle = E_0 |\Phi_0\rangle$$

$$\hat{H}\hat{H}^{-1} = \hat{H}^{-1}\hat{H} = \mathbb{1}$$

$$|\Phi_0\rangle = E_0 \hat{H}^{-1} |\Phi_0\rangle$$

$\hat{H}$ is a differential operator

$\hat{H}^{-1}$ is an integral operator

insert $\int_{-\infty}^{\infty} |\vec{x}\rangle\langle\vec{x}| d\vec{x}$

insert between H and $|\Phi_0\rangle$
and multiply with $\langle y|$

$$\underline{\langle y|\Phi_0\rangle} = \underline{\Phi_0(\vec{y})} = E_0 \int_{-\infty}^{\infty} \langle \vec{y}|H^{-1}|\vec{x}\rangle \times \langle \vec{x}|\Phi_0\rangle d\vec{x}$$

$$\phi_0(\vec{y}) = E_0 \int_{-\infty}^{\infty} \underline{\langle \vec{y}|H^{-1}|\vec{x}\rangle}\, \Phi_0(\vec{x})\, d\vec{x}$$

$$\underline{G(\vec{y},\vec{x}) = \langle y|H^{-1}|x\rangle} \text{ (propagator)}$$

= Green's function

$$\Phi_0(y) = \underline{\hat{H}(\vec{y})\, \hat{H}^{-1} \Phi_0}(\vec{y})$$

$$= \int_{-\infty}^{\infty} \underline{\hat{H}(\vec{y})} G(\vec{y},\vec{x})\, \Phi_0(\vec{x})\, d\vec{x}$$

$$\boxed{\begin{aligned} \hat{H}(\vec{y})\, G(\vec{y},\vec{x}) &= \delta(\vec{y}-\vec{x}) \\ \hat{H}(\vec{x})\, G(\vec{x},\vec{y}) &= \delta(\vec{x}-\vec{y}) \end{aligned}} \Rightarrow$$

$$G(\vec{y},\vec{x}) = G(\vec{x},\vec{y})$$

$$G(\vec{y}\, t|\vec{x}, t-\Delta t) = G(\vec{y},\vec{x},\Delta t) = G(\vec{x},\vec{y},\Delta t)$$

In Metropolis-Hastings

$$\frac{T(i \to j) P_i}{T(j \to i) P_j} \to$$

$$\frac{G(\vec{y}, \vec{x}, \delta t) \, |\psi(\vec{y})|^2}{G(\vec{x}, \vec{y}, \delta t) \, |\psi(\vec{x})|^2}$$

$$= \frac{|\psi(\vec{y})|^2}{|\psi(\vec{x})|^2}$$

- 2nd Digression

Diff eq (1-Dim)

$$P(\vec{x}, t) \to w(x,t)$$

$$\frac{\partial w(x,t)}{\partial t} = D \frac{\partial^2 w(x,t)}{\partial x^2}$$

$$\lim_{t \to 0} w(x,t) \to \delta(x)$$

Fourier transform:

$$w(x,t) = \int_{-\infty}^{\infty} dk \, e^{ikx} \tilde{w}(k,t)$$

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx}$$

$$\tilde{w}(k,0) = \frac{1}{2\pi}$$

Fourier-transformation of diff eq:

$$\frac{\partial \tilde{w}(k,t)}{\partial t} = -Dk^2\tilde{w}(k,t)$$

$$\tilde{w}(k,t) = \underbrace{\tilde{w}(k,0)}_{\frac{1}{2\pi}} e^{-Dk^2t}$$

$$w(x,t) = \int_{-\infty}^{\infty} dk\, \frac{1}{2\pi} e^{ikx} e^{-Dk^2t}$$

$$(k \to k - i\,x/2Dt)$$

$$w(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left\{-\frac{x^2}{4Dt}\right\}$$

$$\int_{-\infty}^{\infty} dx\; w(x,t) = \underline{1}$$

Markov-chain

$$w(x,t) = \int_{-\infty}^{\infty} W(x,t|x_0 t_0)\, w(x_0 t_0) \times dx_0$$

Transition probability

$$\frac{\partial W(x,t|x_0 t_0)}{\partial t} = D \frac{\partial^2}{\partial x^2} W(x t|x_0 t_0)$$

$$W(x t|x_0 t_0) =$$

$$(\Delta t = t - t_0)$$

$$\frac{1}{\sqrt{4\pi D \Delta t}} \exp\left\{\frac{-(x-x_0)^2}{4D\Delta t}\right\}$$

$$\int_{-\infty}^{\infty} dx\, W(x t|x_0 t_0) = \underline{1}$$

Metropolis – Hastings

$$\frac{W(x t|x_0 t_0)\, w(x t)}{W(x_0 t_0|x t)\, w(x_0 t)}$$

$$= \frac{w(x\,t)}{w(x_0\,t)}$$

$\Longrightarrow$ Fokker-Planck

Basic elements in a VMC code;

- Metropolis (plain) ✓
- Analytical expression $E_L(\vec{R};\vec{\alpha})$ ✓
- importance sampling ✓
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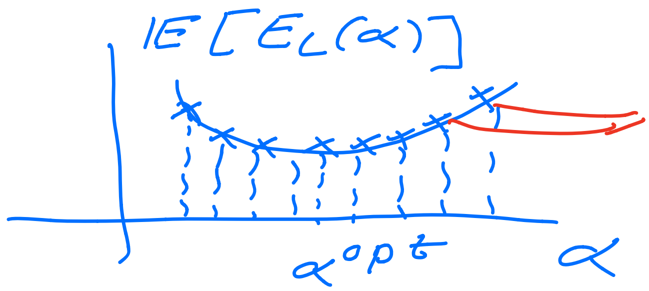


Equally many cycles

$$\alpha^{opt} = \underset{\alpha \in \mathbb{R}^M}{\arg\min}\, \mathbb{E}[E_L(\alpha)]$$

Can we avoid this?

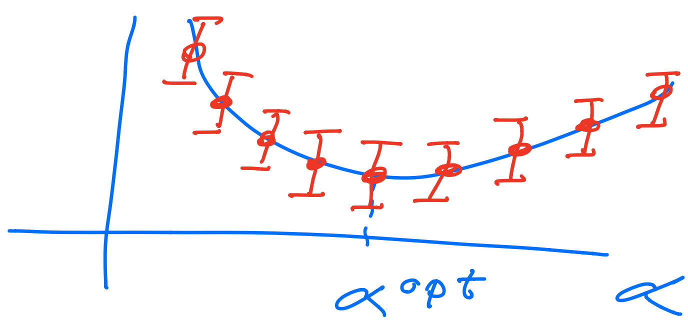
Yes

yes → gradient methods

where we run our full scale VMC calculation

✓ Gradient descent optimization,

✓ Resampling methods



Error estimate – Post analysis $\left\{ \begin{array}{l} \text{Bootstrap} \\ \text{Blocking} \end{array} \right.$

✓ parallelization