FYS 4411/9411

FEB 7, 2025

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Reminder from last week

$$w_i(t) = \sum_j W(j \to i)\, w_j(t')$$

$$\lim_{t \to \infty} w_i(t) = w_i$$

Transition probability

$$\underbrace{\sum_j W(j \to i)}_{\text{unknown}} = 1$$

$$W(j \to i) = \underbrace{T(j \to i)}_{\substack{\text{Prob for} \\ \text{a specific} \\ \text{transition}}} \underbrace{A(j \to i)}_{\substack{\text{acceptance} \\ \text{prob}}}$$

Detailed balance

$$\frac{A(j \Rightarrow i)}{A(i \Rightarrow j)} = \boxed{\frac{w_i}{w_j}} \boxed{\frac{T(i \Rightarrow j)}{T(j \Rightarrow i)}}$$

Known

$T(j \Rightarrow i) = T(i \Rightarrow j)$

Metropolis

$$w_i \rightarrow \frac{|\psi_T(\vec{R}_i; \vec{\alpha})|^2}{\int_{\vec{R} \in D} d\vec{R}\, |\psi_T(\vec{R}; \vec{\alpha})|^2}$$

aside: computational technicality.

(i) move one particle at the time

Ex HO in d-dim and 3 particles

$$\frac{w_i}{w_j} = \frac{e^{-\alpha^2(r_1'^2 + r_2^2 + r_3^2)}}{e^{-\alpha^2(r_1^2 + r_2^2 + r_3^2)}}$$

$$= e^{-\alpha^2(r_1'^2 - r_1^2)}$$

(ii) move all

$$e^{-\alpha^2(r_1'^2 + r_2'^2 + r_3'^2 - r_1^2 - r_2^2 - r_3^2)}$$

Importance sampling =

Model for $T(i \to j)$, based on $\Psi_T(\vec{R}_i; \vec{\alpha})$

Metropolis Test

$$A(j \to i) = \min\left(1, \frac{w_i T(i \to j)}{w_j T(j \to i)}\right)$$

Basics of Monte Carlo (Stochastic) integration.

$$I = \int_0^1 f(x)\,dx$$

Uniform distribution - U

$X \sim U$

$$p(x)\,dx = \begin{cases} dx & 0 \le x \le 1 \\ 0 & \text{else} \end{cases}$$

M = # of samples

$M = 1000$, with Uniform PDF

$\underbrace{0 \to 0.1}_{100}$; $\underbrace{0.1 \to 0.2}_{100}$, ...

$$I = \int_0^1 f(x)\,dx = \int_0^1 p(x) f(x)\,dx$$

$$\left(\boxed{\int_0^1 p(x)\,dx = 1} \right) = \mathbb{E}[f(x)]$$

$$\int_{-\infty}^{\infty} p(x)\,dx = 1 \qquad 0 \leq p(x) \leq 1$$

$$\int_{-\infty}^{a} p(x)\,dx \leq \int_{-\infty}^{b} p(x)\,dx$$

$$a \leq b$$

(i) change of variable
[RNG are based on uniform PDF]

(ii) importance sampling

change of variable

Ex 1

$$p(y)\,dy = e^{-y}\,dy \qquad y \in [0,\infty)$$

conservation of probability

$$p(y)\,dy = p'(x)\,dx$$

$$\underbrace{p'(x)\,dx}_{\text{uniform}} = dx \qquad x \in [0,1]$$

$$p(y)\,dy = e^{-y}\,dy = dx$$

$$y \in [0, \infty)$$

$$x(y) = \int_0^y e^{-y'}\,dy'$$

$$= 1 - e^{-y} \Rightarrow$$

$$y(x) = -\ln(1-x)$$

$y = 0$ when $x = 0$ $\wedge$ $y = \infty$ when $x = 1$

Ex 2

$$p(x) = \frac{1}{3}(4-2x) \quad x \in [0,1]$$

$$\int_0^1 p(x)\,dx = \underline{1}$$

$p(y)\,dy$ is a uniform PDF

$$y \sim U \qquad y \in [0,1]$$

$$y(x) = \frac{1}{3}(4-x)x \Rightarrow x(y)$$

$y = 0$ when $x = 0$

$y = 1$ when $x = \underline{1}$

why ?

(ii) importance sampling

$$I = \int_0^1 \frac{dx}{1+x^2} = \frac{\pi}{4}$$

$$\int f(x)\,dx$$

$$= \int_0^1 p(x)\,\frac{f(x)}{p(x)}\,dx$$

$$p(x) = \frac{1}{3}(4-2x)$$

$$\frac{f(0)}{p(0)} = \frac{f(1)}{p(1)} = 3/4$$

(constant)

The ideal is that $\frac{f(x)}{p(x)} =$ constant for all x

$$I = \int_0^1 p(x) \boxed{\frac{f(x)}{p(x)}} dx$$

$F(x)$ if const

$$I = \int_0^1 p(x)\, F(x)\, dx = \text{const} \underbrace{\int_0^1 p(x) dx}_{=1}$$

$$\mathbb{E}[F(x)] = \int_0^1 p(x)\, F(x)\, dx$$

$$\text{var}[F(x)] = \int_0^1 p(x) \left[F(x) - \mathbb{E}[F(x)]\right]^2 \times dx$$

$$= \int_0^1 p(x)\, F^2(x)\, dx - \left(\mathbb{E}[F]\right)^2 = 0$$

if const

with zero variance, then STD is also zero

with a change of variables

$$p(y)\,dy = dy = \frac{1}{3}(4-2x)\,dx$$

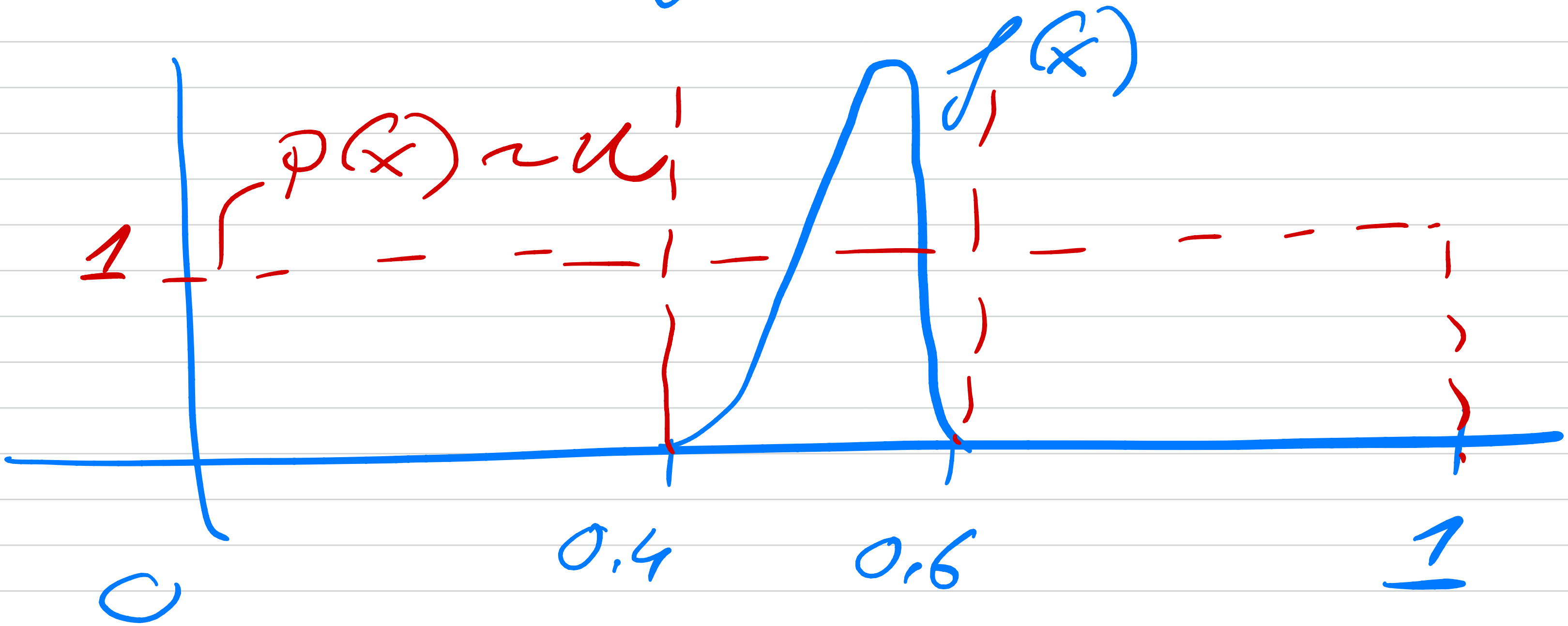
$$I = \int_0^1 p(x)\,\frac{f(x)}{p(x)}\,dx$$

RNG ~ U

$$= \int_0^1 \frac{f(x(y))}{p(x(y))}\,dy$$

$$p(x)\,dx = dy$$

Ex 3 $\quad f(x) \quad x \in [0, 1]$



$$I = \int_0^1 f(x)\,dx \simeq \frac{1}{M} \sum_{i=1}^{M} f(x_i)$$

$M = 1000$

only 200

are in

$x \in [0.4, 0.6]$

ideal: find a PDF $p'(y)$

$y \in [0.4, 0.6]$ where $f(x)$

is nonzero [change of variable part]

then have $\dfrac{f(y)}{p'(y)} \approx \text{const}$

in this case [importance sampling]

$\mathrm{var}[f] \approx 0$ (small)

Ansatz for Ψ_T

$$E_L(\vec{R}) = \frac{1}{\Psi_T(\vec{R})} \hat{H} \Psi_T(\vec{R})$$

electron in atomic hydrogen.

in spherical coordinates

$$\Psi_{nl}(r,\theta,\varphi) = R_{nl}(r) Y_{lm_l}(\theta,\varphi)$$

$$r \in [0, \infty)$$

$$\theta \in [0, \pi]$$

$$\varphi \in [0, 2\pi]$$

$\hat{H}$ (in atomic units)

$$\hat{H} = -\frac{1}{2}\nabla^2 - \frac{1}{r}$$

Local energy for the radial part

$$E_L(r) = \frac{1}{R_T(r)}\left(-\frac{1}{2}\frac{d^2}{dr^2} - \boxed{\frac{1}{r}}\frac{d}{dr} - \boxed{\frac{1}{r}}\right)$$

$$\times R_T(r) + \text{finite terms}$$

$$\lim_{r \to 0} \frac{d^n R_T}{dr^n} = L < \infty \quad (\sigma, \varphi)$$

$$\lim_{r \to 0} E_l(r) = \underbrace{\frac{1}{R_T}\left(-\frac{1}{r}\frac{d}{dr} - \frac{1}{r}\right)R_T}_{} = 0$$

(omitted finite terms)

$$\frac{dR_T}{dr} = -R_T \Rightarrow$$

$$R_T = e^{-r}$$ Minimal requirement

$$R_{nl}(r) = e^{-\alpha r} \underline{L_{nl}(r)}$$ Laguerre

For potentials like

$$\frac{1}{|\vec{r}_1-\vec{r}_2|} = \frac{1}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}}$$

For two particles getting close to each other

$\lim_{|\vec{r}_1-\vec{r}_2|} = 0 \Rightarrow$ term in relative kinetic energy which cancels $\frac{1}{|\vec{r}_1-\vec{r}_2|} \Rightarrow$

$$R_T(r_1, r_2) \approx e^{\beta r_{12}} \qquad r_{12} = |\vec{r}_1-\vec{r}_2|$$

ansatz for atomic helium

$$\Psi_T(\vec{r}_1, \vec{r}_2) \propto \underbrace{e^{-\alpha(r_1+r_2)}}_{\text{one body}} \; \underbrace{e^{\beta r_{12}}}_{\text{corre-lated part}}$$

Jastrow function

HO for two electrons in 2d.

$n_x = n_y = 0$

$$\Psi_T(\vec{r}_1, \vec{r}_2) = e^{-\alpha^2(r_1^2 + r_2^2)} \, e^{\beta r_{12}}$$

$$\vec{r}_1 = \vec{e}_x x_1 + \vec{e}_y y_1$$

variational parameter