بسم الله الرحمن الرحیم

جلسه ۷ / ۱۰ / ۱۴۰۰

* Hamiltonian Monte Carlo ②

MCMC $\quad \{\theta\}_{old} \longrightarrow \{\theta\}_{New}$

$$P(\{\theta\}|D) \sim \mathcal{L}(\{D\}|\{\theta\})\, P(\{\theta\})$$

if $P(\{\theta\}) = cts$ and according to Conteral limit theorem

$$\mathcal{L} \sim e^{-\chi^2/2} \longrightarrow \frac{\mathcal{L}_{New}}{\mathcal{L}_{old}}$$

Acceptance Rate

پارامتر کمکی که نقش اندازه حرکت

$$\chi^2(\{\theta\}) \longrightarrow \mathcal{H}(\{\theta\},\{u\})$$

model free parameters

auxiliary Conjugate momentum

$$\mathcal{H}(\{\theta\},\{u\}) = K(\{u\}) + V(\{\theta\})$$

phenomenological approach

$$\text{Hamiltonian} = \underbrace{K(\{u\})}_{\text{Kinetic Part}} + \underbrace{\frac{\chi^2(\{\theta\})}{2}}_{\text{Potential Part}}$$

$$K(\{u\}) = \frac{\vec{u}^T \vec{u}}{2}$$

a Simple form

Centeral limit Theorem

$\{u\} = \{u_1, u_2 \dots u_M\}$

$\{\theta\} = \{\theta_1 \dots \theta_M\}$

Conjugate momentum

model Free Parameter

$\mathcal{N}(0, 1)$ = Multivarsate Gaussian models

mean valu

$\langle u \rangle = 0$

$\sigma_u^2 = 1$

$$\{u\} = \{\dot{\theta}\}$$

$$\left.\begin{aligned} \frac{\partial \{u\}}{\partial t} &= -\frac{\partial \mathcal{H}}{\partial \{\theta\}} \\ \frac{\partial \{\theta\}}{\partial t} &= \frac{\partial \mathcal{H}}{\partial \{u\}} \end{aligned}\right\}$$

$\boxed{\text{Equation of Evolution}}$

$$\frac{\partial \{u\}}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \{\theta\}} = -\frac{\partial \chi^2}{\partial \{\theta\}}$$

Force

> 0

< 0

$$\chi^2(\{\theta\}) \longrightarrow \chi^2_{min}(\{\theta\}_{Best})$$

$$\mathcal{H}(\{\theta\},\{u\}) \longrightarrow \mathcal{H}_{min}(\{\theta\}_{Best}, \{u\}_{\cancel{Best}})$$

پارامترهای کمکی هستند

Therefore

$$\mathcal{L}(\{D\}|\{\theta\}) = e^{-\frac{\chi^2(\{\theta\})}{2}}$$

$$\mathcal{H}(\{\theta\},\{u\})$$

$$\mathcal{L}(\{D\}|\{\theta\}) = e^{-\mathcal{H}(\{\theta\},\{u\})}$$

$$\boxed{\mathcal{L}(\{D\}|\{\theta\}) = e^{-\frac{\chi^2(\{\theta\})}{2}} \mathcal{N}_u(0,1)}$$

$$\mathcal{L} = e^{-\frac{\chi^2(\{\theta\})}{2} + K(\{u\})}$$

HMC Algorithm

Import Data $\{D\}$

Select $\underbrace{\{\theta\}_{old}}$ and $\{u\}_{old} : \mathcal{N}(u,0,1)$

Compute $\chi^2_{old}(\{\theta\}_{old})$

$$\mathcal{H}_{old} = \frac{\chi^2_{old}}{2} + \frac{\{u\}^T_{old}\{u\}_{old}}{2}$$

$$\mathcal{L}_{old} = e^{-\mathcal{H}_{old}} = \mathcal{L}_{old}(\{D\}|\{\theta\}_{old})\, \mathcal{N}(u,0,1)$$

MCMC Algorithm

Import Data $\{D\}$

Select $\underbrace{\{\theta\}_{old}}$

Compute $\chi^2_{old}(\{\theta\}_{old})$

$$'' = e^{-\frac{\chi^2_{old}(\{\theta\}_{old})}{2}} \mathcal{N}(u,0,1)$$

این رابطه بطور کلی ممکن است درست نباشد

عددی

loop on MC (Sampling loop) $\rightarrow \mathcal{O}(M')$

- loop on HMC

$$\{\theta\}_{old} \rightarrow \{\theta\}_{old}^{HMC}$$

$$\{u\}_{old} \rightarrow \{u\}_{old}^{HMC}$$

$\mathcal{O}(M'')$

Leapfrog method or Verlet method

- End loop

$$\{\theta\}_{New} = \{\theta\}_{old}^{HMC}$$

$$\{u\}_{New} = \{u\}_{old}^{HMC}$$

Compute $\mathcal{H}_{New}(\{\theta\}_{New}, \{u\}_{New})$

$$\Delta\mathcal{H} = \mathcal{H}_{New} - \mathcal{H}_{old}$$

check acceptance Rate

$$R = \min\{1, e^{-\Delta\mathcal{H}}\}$$

$$\{\theta\}_{old} = \{\theta\}_{New}, \quad \chi^2_{old} = \chi^2_{New}$$

$$\{u\}_{old} = \mathcal{N}(u,0,1)$$ Box Muller

Write $\{\theta\}_{old}, \chi^2_{old}$

End loop MC

$\mathcal{O}(M'M'')$

$\mathcal{O}(M)$

loop on MC (Sampling loop)

$$\{\theta\}_{old} \longrightarrow \{\theta\}_{New}$$

$$\{\theta\}_{New} = \{\theta\}_{old} + \{\Delta\theta\}$$

$$\mathcal{N}(\{\Delta\theta\}, 0, \sigma_{\{\theta\}})$$

آزمون و خطا انتخاب می‌شود.

Compute $\chi^2_{New}(\{\theta\}_{New})$

$$\Delta\chi^2 = \chi^2_{New}(\{\theta\}_{New}) - \chi^2_{old}(\{\theta\}_{old})$$

check acceptance Rate

$$R = \min\{1, e^{-\frac{\Delta\chi^2}{2}}\}$$

$$\{\theta\}_{old} = \{\theta\}_{New}, \quad \chi^2_{old} = \chi^2_{New}$$

write $\{\theta\}_{old}, \chi^2_{old}$

End loop MC

$\mathcal{O}(M)$

if $M' = M$, $M'' = \frac{M}{2}$ $\rightarrow$ HMC $\mathcal{O}\left(\frac{M^2}{2}\right)$; MCM $\mathcal{O}(M)$

$$\mathcal{O}\left(\frac{M^2}{2}\right) > \mathcal{O}(M)$$

HMC Speed < MCMC speed ?!

$$\underbrace{\underbrace{\mathcal{O}(M'M'')}_{HMC} \ll \underbrace{\mathcal{O}(M)}_{MCMC}}$$

Model free paremter $N \gg 1$

تعداد پارامترهای مدل زیاد بشود [illegible] اما در کت ترا[illegible]

HMC loop

loop $j = 1, M''$ — Verlet algorithm

$x \rightarrow \{\theta\}^{j+1}_{old} = \{\theta\}^{j}_{old} + \{u\}^{j}_{old}\,\epsilon + \frac{1}{2}\epsilon^2\left(-\frac{\partial \mathcal{H}}{\partial \{\theta\}^{j}_{old}}\right)$

$v \rightarrow \{u\}^{j+1}_{old} = \{u\}^{j}_{old} + \frac{1}{2}\underbrace{\left\{-\frac{\partial \mathcal{H}}{\partial\{\theta\}^{j+1}_{old}} - \frac{\partial \mathcal{H}}{\partial\{\theta\}^{j}_{old}}\right\}}\epsilon$

در جزییات بیشتر [illegible]

HMC

$$\frac{\partial u}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \theta}$$

$$\frac{u(t+\Delta t) - u(t)}{\Delta t} = -\frac{\partial \mathcal{H}}{\partial \theta} \;-\; u(t+\Delta t) = u(t) + \Delta t\left(-\frac{\partial \mathcal{H}}{\partial \theta}\right)$$

End loop

Leapfrog algorithm

$$\boxed{\frac{\partial \mathcal{H}}{\partial \theta} = \frac{\mathcal{H}(\theta+\Delta\theta) - \mathcal{H}(\theta)}{\Delta\theta}}$$

HMC

loop $j=1,\ M''$

$$\{u\}_{old}^{j+1/2} = \{u\}_{old}^{j} - \frac{\epsilon}{2}\,\frac{\partial \mathcal{H}}{\partial \{\theta\}_{old}^{j}}$$

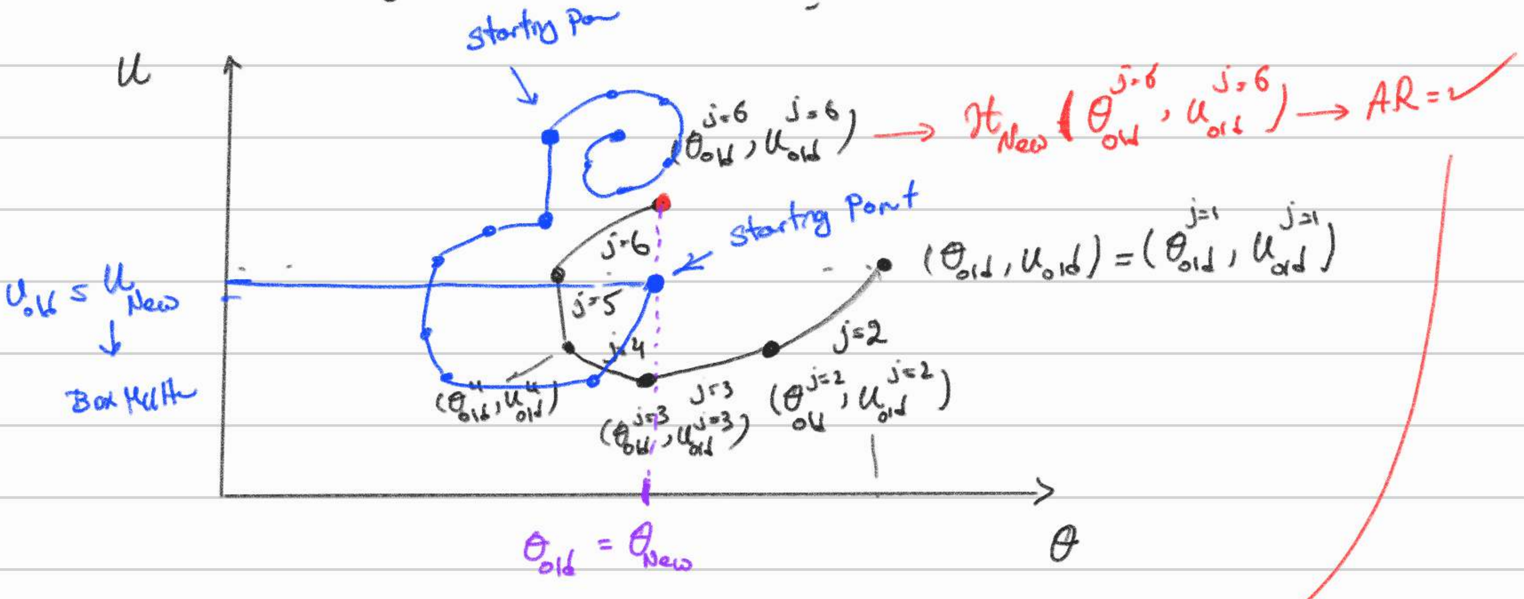
$$\{\theta\}_{old}^{j+1} = \{\theta\}_{old}^{j} + \epsilon\,\{u\}_{old}^{j+1/2}$$

$$\{u\}_{old}^{j+1} = \{u\}_{old}^{j} - \frac{\epsilon}{2}\,\frac{\partial \mathcal{H}}{\partial \{\theta\}_{old}^{j+1}}$$

End loop

A schematic presentation of Sobroutin HMC

$M''=6$ $\quad j=1,\ 6$ $\quad$ فرض کنید.

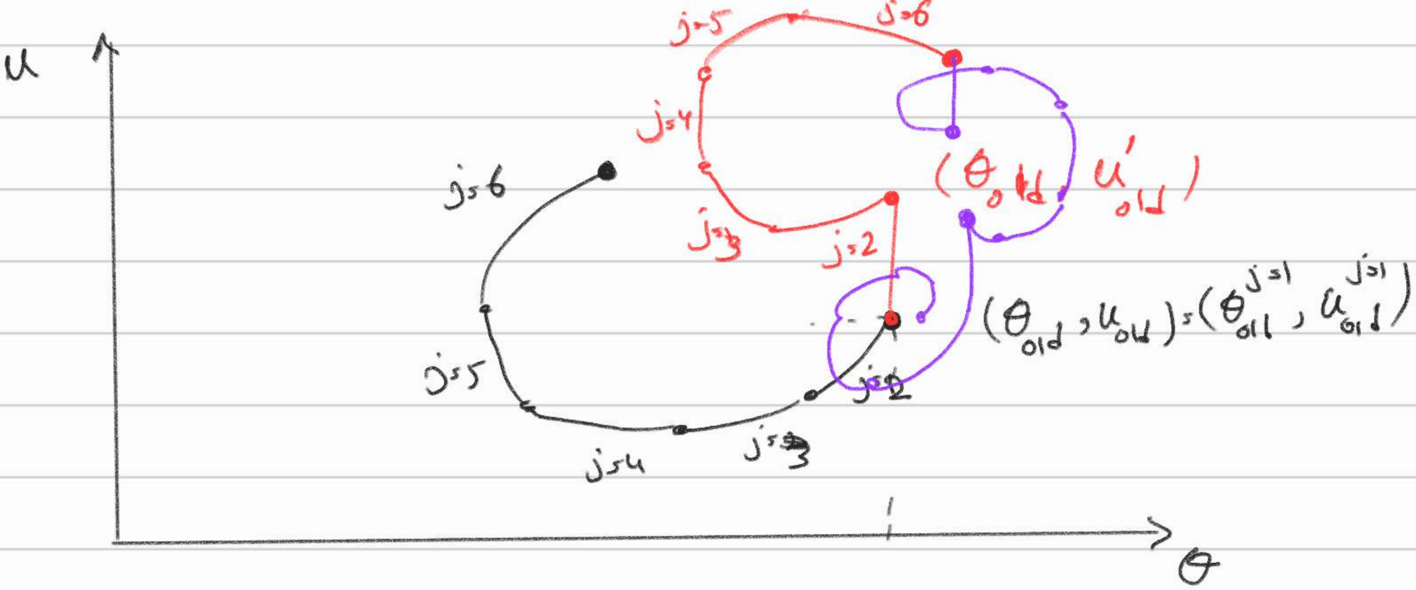


$$\theta_{old} = \theta_{New} = \theta_{old}^{j=6}$$

انتخاب می‌شود

$AR = ✓$

$\theta_{old} \longleftarrow \theta_{New} = ✓$



شرط همگرایی قابل تعریف است.

$R < 1.0$