Monte Carlo

martes, 2 de marzo de 2021 14:04

How to perform Monte Carlo.

$p(\vec{s})$: complicated dist.
from which you would like to extract
eq. conf

Monte - Carlo: it is a stochastic process.
Here, starting from a rdm conf $\vec{s}_0$
we generate randomly a seq. of new conf

$$\vec{s}_0 \longrightarrow \vec{s}_1 \longrightarrow s_2 \longrightarrow \dots \longrightarrow s_T$$

and eventually, when T is large you
hope that s_T is a "typical" conf from $p(\vec{s})$

I) Single spin-flip dynamics.

$$P(\vec{s},t+1) = \sum_{\vec{s}'} W(\vec{s}' \to \vec{s}) P(\vec{s}',t) - \sum_{\vec{s}' \neq \vec{s}} W(\vec{s} \to \vec{s}') P(\vec{s},t)$$

$$\cancel{P(\vec{s},t)} + \Delta t \frac{\partial P(\vec{s},t)}{\partial t} = \quad " \quad " \quad "$$

stat dist: $\frac{\partial P}{\partial t} = 0 = \sum_{\vec{s}} \left(\underbrace{W(\vec{s}' \to \vec{s}) P_q(\vec{s}')} - \underbrace{W(\vec{s} \to \vec{s}') P_q(\vec{s})} \right)$

stat distr: $\frac{\partial P}{\partial t} = 0 = \sum_{\vec s'} \underbrace{\left(W(\vec s' \to \vec s) P_{eq}(\vec s') - W(\vec s \to \vec s') P_{eq}(\vec s) \right)}_{=0}$

$$\frac{W(\vec s' \to \vec s)}{W(\vec s \to \vec s')} = \frac{P_{eq}(\vec s)}{P_{eq}(\vec s')}$$: detailed balance cdt

find W that sat this eq.

Two well-known dynamics

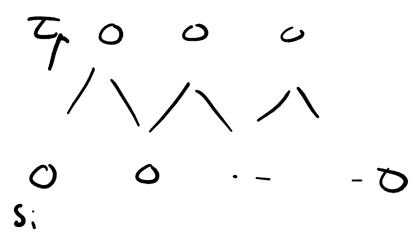
i) Heat-bath: ∃ take i : $p(s_i | \vec s_{\setminus i}) = \dfrac{e^{\beta \overbrace{[E(s_i) - E(-s_i)]}^{\Delta E}}}{2ch(\beta \Delta E)}$

ii) Glauber dynamics. $s_i = \begin{cases} -s_i & \text{if the energy is reduced by this move} \end{cases}$

$\begin{cases} -s_i & \text{with } \sim e^{-\beta \Delta E} \\ s_i & \text{with } \sim 1 - e^{-\beta \Delta E} \end{cases}$

In the case of a bipartite network we can use the following trick

$$\mathcal{H} = -\sum_{i,\mu} s_i \xi_i^\mu \tau_\mu$$



you can show that

· $p(\vec\tau | \vec s) = \prod_\mu p(\tau_\mu | \vec s)$

· $p(\vec s | \vec \tau) = \prod_i p(s_i | \vec \tau)$

this means that in Hopfield

$p(\tau_\mu | \vec s)$ → is a gaussian

$p(s_i | \vec\tau)$ → is a bernoulli

you can use the following dynamics:

$$\vec{s}_0 \longrightarrow \vec{\tau}_0 \sim p(\vec{\tau}|\vec{s}_0) \longrightarrow \vec{s}_1 \sim p(\vec{s}|\tau_0)$$

$$\dots \qquad \vec{s}_T \sim p(\vec{s}|\tau_{T-1})$$

At the end you obtain: $\{\vec{s}_T, \vec{\tau}_T\}$: an equilibrated conf.

Remind: $p(\vec{s},\vec{\tau}) \propto \exp\left(\sum_{i,\mu} s_i \xi_i^\mu \tau_\mu\right) \cdot e^{-\sum_\mu \frac{\tau_\mu^2}{2}}$

$$\begin{cases} \xi : \mathbb{R}^{P \times N_v} & N_v : \# \text{ of vis. var} \\ V : \mathbb{R}^{N_v \times N_s}, & N_s \text{ is the } \# \text{ of samples} \\ H : \mathbb{R}^{P \times N_s}; \end{cases}$$

$$\beta H = -\frac{\beta}{2N} \sum_\mu \left(\sum_i s_i \xi_i^\mu\right)^2$$

$$\Big\} \boxed{\beta' = \sqrt{\beta}}$$

$$\beta' H = \sqrt{\frac{\beta}{N}} \sum_{i,\mu} s_i \xi_i^\mu \tau_\mu$$

$\boxed{\xi' = \sqrt{\frac{\beta}{N}}\xi}$

1) $p(s_i|\vec{\tau})$: $$p(\vec{s}|\vec{\tau}) \overset{\text{Bayes}}{=} \frac{p(\vec{s},\vec{\tau})}{p(\vec{\tau})} = \frac{e^{\cancel{-\sum_\mu \frac{\tau_\mu^2}{2}} + \sum_{i,\mu} s_i \xi_i'^\mu \tau_\mu}}{\cancel{Z} \cdot \sum_{\{s\}} \cancel{e^{-\sum_\mu \frac{\tau_\mu^2}{2}}} + \sum_{i,\mu} s_i \xi_i'^\mu \tau_\mu} \cdot \cancel{Z}$$

where $p(\vec{\tau}) = \sum_{\{s\}} p(\vec{s},\vec{\tau})$

$$= \frac{\prod_i \left[\exp\left(s_i \sum_\mu \xi_i'^\mu \tau_\mu\right)\right]}{\prod_i \left[\sum_{s_i=\pm 1} \exp\left(s_i \sum_\mu \xi_i'^\mu \tau_\mu\right)\right]} = \prod_i \left[\frac{e^{s_i \sum_\mu \xi_i'^\mu \tau_\mu}}{2 \cdot \mathrm{ch}\left(\sum_\mu \xi_i'^\mu \tau_\mu\right)}\right]$$

$s_i \sum_\mu \xi_i'^\mu \tau_\mu$

from the factorization, we have that $p(s_i|\vec{\tau}) = \dfrac{e^{s_i \sum_\mu \xi_i^{\mu'} \tau_\mu}}{2\,\mathrm{ch}\left(\sum_\mu \xi_i^{\mu'} \tau_\mu\right)}$

$$\boxed{\langle s_i \rangle_{p(s_i|\vec{\tau})} = \mathrm{th}\left(\sum_\mu \xi_i^{\mu'} \tau_\mu\right)} = \mathrm{th}\left(\sqrt{\frac{\beta}{N}} \sum_\mu \xi_i^\mu \tau_\mu\right)$$

ii) $$p(\vec{\tau}|\vec{s}) = \frac{\prod_\mu \left[e^{-\frac{\tau_\mu^2}{2} + \sum_i \xi_i^{\mu'} s_i} \right]}{\prod_\mu \int d\tau_\mu \, e^{-\frac{\tau_\mu^2}{2} + \sum_i \xi_i^{\mu'} s_i}} \longrightarrow p(\tau_\mu|\vec{s}) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\tau_\mu - \sum_i \xi_i^{\mu'} s_i\right)^2\right]$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\tau_\mu - \sqrt{\frac{\beta}{N}} \sum_i \xi_i^\mu s_i\right)^2\right]$$

$$\boxed{\langle \tau_\mu \rangle_{p(\tau_\mu|\vec{s})} = \sqrt{\frac{\beta}{N}} \sum_i \xi_i^\mu s_i}$$

Sample Hidden: $p(\tau_\mu|\vec{s})$, $\forall \mu$, $\to \langle \tau_\mu \rangle$

$\hookrightarrow$ generate sample $\tau_\mu \sim p(\tau_\mu|\vec{s})$

np.random.normal(list_mean_τ)
$\mathbb{R}^{P \times N_s}$

Sample Vis. $\langle s_i \rangle$: $p(s_i = +1|\vec{\tau}) = \dfrac{\langle s_i \rangle + 1}{2}$

$\to$ np.random.rand(..) $<$ $p(s_i = +1)$

Sampling. $V \leftarrow$ rdm init. conf.
for t in range(tmax):
~100/500
$H_i(\text{Hid}) \leftarrow$ SampleHidd(V)

$H_i(\Pi H) \longleftarrow \text{SampleHidd}(V)$

$V_i(\Pi V) \longleftarrow \text{SampleVis}(H)$