TP1: Reminder on Markov Chains - Stochastic gradient descent

Exercice 1: Box-Muller and Marsaglia-Bray algorithm

1. Let $f: \mathbb{R}^2 \to \mathbb{R}$ integrable.

We note $\phi: (r, \theta) \in \mathbb{R}_+^* \times]0, 2\pi [\mapsto (r\cos\theta, r\sin\theta) \in \mathbb{R}^2 - \{(0, x), x \ge 0\}, \text{ which is a diffeomorphism, we can apply the change of variable theorem with } (x, y) = (r\cos\theta, r\sin\theta). On a det <math>J_{\phi} = r$.

$$\mathbb{E}[f(X,Y)] = \mathbb{E}[f(\phi(R,\Theta))]$$

$$= \frac{1}{2\pi} \int_{\mathbb{R}_{+}^{*} \times]0,2\pi[} f(r\cos\theta, r\sin\theta) r e^{-\frac{r^{2}}{2}} dr d\theta$$

$$= \frac{1}{2\pi} \int_{\mathbb{R}^{2} - \{(0,x),x \geqslant 0\}} f(x,y) e^{-(x^{2} + y^{2})/2} dx dy$$

$$= \frac{1}{2\pi} \int_{\mathbb{R}^{2}} f(x,y) e^{-(x^{2} + y^{2})/2} dx dy$$

We deduce the p.d.f of couple (X,Y) which is $f_{X,Y}(x,y) = \frac{1}{2\pi}e^{-\frac{x^2+y^2}{2}} = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}\frac{1}{\sqrt{2\pi}}e^{-\frac{y^2}{2}} = f_X(x)f_Y(y)$. We showed that $X,Y \sim \mathcal{N}(0,1)$ and the independence of variables X and Y.

2. The previous question show that if we know how to generate a uniform variable Θ , on $[0, 2\pi]$, and a Rayleigh variable R, which are independent, then we know how to simulate two independent variables of distribution $\mathcal{N}(0,1)$.

The Python language allows us to generate a uniform distribution on [0,1], hence on $[0,2\pi]$. Let's proof that we can simulate a Rayleigh variable by Inverse transform sampling.

Let R be a Rayleigh variable. We have

$$F_R(x) = \mathbb{P}(R \leqslant x) = \int_0^x re^{-\frac{-r^2}{2}} dr = \left[-e^{-\frac{r^2}{2}} \right]_0^x = 1 - e^{\frac{-x^2}{2}}$$

This c.d.f is invertible of inverse $F_R^{-1}(y) = \sqrt{-2\ln(1-y)}$.

Algorithm 1 Sampling independent gaussian variables

Sample independent random variables $U_1, U_2 \sim \mathcal{U}([0,1])$.

 $\Theta \leftarrow 2\pi U_1$

 $R \leftarrow \sqrt{-2\ln\left(1 - U_2\right)}$

 $X \leftarrow R \cos \Theta$

 $Y \leftarrow R \sin \Theta$

Output: X, Y

3. (a) The while loop correspond to a rejection sampling. The target distribution is the uniform distribution on the unit disk (of p.d.f $\frac{1}{\pi} \mathbb{1}_{D(0,1)}$), and the distribution that we know how to generate is the uniforme distribution on square $[-1,1]^2$ of p.d.f $\frac{1}{4} \mathbb{1}_{[-1,1]^2}$). Hence, the random couple (V_1, V_2) follows a uniform distribution on the unit disk.

Let's proof that rigorously. For sake of clarity, we'll denote $V_{i,1}, V_{i,2}$ the variables generated at the i-th step of the loop.

Let
$$T = \inf \{ i \in \mathbb{N}^*, V_{i,1}^2 + V_{i,2}^2 \le 1 \}.$$

We want to show that $(V_{T,1}, V_{T,2})$ follows a uniform distribution on the unit disk.

Let $f: [-1,1]^2 \to \mathbb{R}$ a bounded and measurable function.

We have:

$$\mathbb{E}[f(V_{T,1}, V_{T,2})] = \mathbb{E}\left[\sum_{k=1}^{\infty} f(V_{k,1}, V_{k,2}) \, \mathbbm{1}_{(T=k)}\right]$$

$$= \sum_{k=1}^{\infty} \mathbb{E}[f(V_{k,1}, V_{k,2}) \, \mathbbm{1}_{(V_{k,1}^2 + V_{k,2}^2 \leqslant 1)} \prod_{i < k} \mathbbm{1}_{(V_{i,1}^2 + V_{i,2}^2 > 1)}]$$

$$= \sum_{k=1}^{\infty} \mathbb{E}[f(V_{k,1}, V_{k,2}) \, \mathbbm{1}_{(V_{k,1}^2 + V_{k,2}^2 \leqslant 1)}] \left(1 - \frac{\pi}{4}\right)^{k-1} \text{ by independence}$$

$$= \frac{4}{\pi} \frac{1}{4} \int_{[-1,1]^2} f(v_1, v_2) \, \mathbbm{1}_{v_1^2 + v_2^2 \leqslant 1} \, \mathrm{d}v_1 \, \mathrm{d}v_2$$

$$= \frac{1}{\pi} \int_{D(0,1)} f(v_1, v_2) \, \mathrm{d}v_1 \, \mathrm{d}v_2$$

(b) Let $f:[0,1]^2 \to \mathbb{R}, g:[0,1] \to \mathbb{R}$ bounded, measurable. We show, by using the diffeomorphisme $\phi:(v,\theta)\in]0,1[\times]0,2\pi[\mapsto (\sqrt{v}\sin\theta,\sqrt{v}\cos\theta)\in D(0,1)$ of inverse $\phi^{-1}(v_1,v_2)=\left(v_1^2+v_2^2,2\arctan\left(\frac{v_2}{\sqrt{v_1^2+v_2^2}+v_1}\right)\right)$ and such that $|\det J(\phi)(v,\theta)|=1/2$, and by applying the change of variable theorem with $(v_1,v_2)=(\sqrt{v}\cos\theta,\sqrt{v}\sin\theta)$, that :

$$\mathbb{E}[f(T_1, T_2)] = \frac{1}{\pi} \int_{D(0,1)} f\left(\frac{v_1}{\sqrt{v_1^2 + v_2^2}}, \frac{v_2}{\sqrt{v_1^2 + v_2^2}}\right) dv_1 dv_2$$

$$= \frac{1}{\pi} \int_0^1 \int_0^{2\pi} f(\cos \theta, \sin \theta) |\det J(\phi)(v, \theta)| d\theta dv$$

$$= \frac{1}{2\pi} \int_0^{2\pi} f(\cos \theta, \sin \theta) d\theta$$

et

$$\mathbb{E}[g(V)] = \frac{1}{\pi} \int_{D(0,1)} g(v_1^2 + v_2^2) dv_1 dv_2$$

$$= \frac{1}{\pi} \int_0^1 \int_0^{2\pi} g(v) |\det J(\phi)(v,\theta)| d\theta dv$$

$$= \int_0^1 g(v) dv$$

Hence, $V \sim \mathcal{U}([0,1])$ and $(T_1, T_2) \sim (\cos \Theta, \sin \Theta)$ where $\Theta \sim \mathcal{U}([0,2\pi])$.

$$\mathbb{E}[f(T_1, T_2)g(V)] = \mathbb{E}\left[f\left(\frac{V_1}{\sqrt{V_1^2 + V_2^2}}, \frac{V_2}{\sqrt{V_1^2 + V_2^2}}\right) g\left(\sqrt{V_1^2 + V_2^2}\right)\right]$$

$$= \frac{1}{\pi} \int_{D(0,1)} f\left(\frac{v_1}{\sqrt{v_1^2 + v_2^2}}, \frac{v_2}{\sqrt{v_1^2 + v_2^2}}\right) g\left(v_1^2 + v_2^2\right) dv_1 dv_2$$

$$= \frac{1}{\pi} \int_{]0,1[\times]0,2\pi[} f(\cos\theta, \sin\theta)g(v) |\det J(\phi)(v,\theta)| dv d\theta$$

$$= \frac{1}{2\pi} \int_0^{2\pi} f(\cos\theta, \sin\theta) d\theta \int_0^1 g(v) dv$$

$$= \mathbb{E}[f(T_1, T_2)] \mathbb{E}[g(V)]$$

The couple (T_1, T_2) and the variable V are independent.

(c) Let's show that S follows a Rayleigh distribution. Let $s \ge 0$.

$$\mathbb{P}(S \leqslant s) = \mathbb{P}(\sqrt{-2\log V} \leqslant s) = \mathbb{P}(V \geqslant e^{-s^2/2}) = 1 - e^{-s^2/2}.$$

The c.d.f of S is the c.d.f of a Rayleigh distribution. According to question 1, the couple $(X, Y) = (ST_1, ST_2)$ follows a multivariate gaussian distribution $\mathcal{N}(0, I_2)$.

(d) We are looking for $\mathbb{E}[T]$ where T is the stopping time defined at question 3. (a) The variable T follows a geometric distribution $\mathcal{G}\left(\frac{\pi}{4}\right)$, then we deduce that $\mathbb{E}[T] = \frac{4}{\pi}$.

Exercice 2: Invariant distribution

Let $I = \left\{ \frac{1}{m}, m \in \mathbb{N}^* \right\}$.

1. The definition of $\mathcal{L}(X_{n+1}|X_n)$ is equivalent to define implicitely a sequence of independant random variable $(Z_{n,m})_{n,m}$ of distribution $\mathcal{B}\left(\frac{1}{m}\right)$ such that $Z_{n,m}$ is independante of X_n and :

$$\begin{cases} X_{n+1} &= \frac{1}{m+1} \text{ si } X_n = \frac{1}{m} \text{ et } Z_{n,m} = 1\\ X_{n+1} &\sim \mathcal{U}([0,1]) \text{ sinon} \end{cases}$$

We have

$$\mathbb{P}[X_{n+1} \in A | X_n \notin I] = \int_{A \cap [0,1]} \mathrm{d}t$$

and

$$\mathbb{P}\left[X_{n+1} \in A | X_n = \frac{1}{m}\right] = \mathbb{P}[Z_{n,m} = 1] \mathbb{P}\left[X_{n+1} \in A | X_n = \frac{1}{m}, Z_{n,m} = 1\right]$$

$$+ \mathbb{P}[Z_{n,m} = 0] \mathbb{P}\left[X_{n+1} \in A | X_n = \frac{1}{m}, Z_{n,m} = 0\right]$$

$$= \frac{1}{m^2} \delta_{\frac{1}{m+1}}(A) + \left(1 - \frac{1}{m}\right)^2 \int_{A \cap [0,1]} dt$$

We deduce the transition kernel of the Markov chain.

2. Let $A \in \mathcal{B}([0,1])$.

We have:

$$P(x,A) = \mathbb{1}_{x \notin I} \pi(A) + \sum_{m=1}^{+\infty} \mathbb{1}_{x=1/m} \left(x^2 \pi(A) + (1-x^2) \delta_{\frac{1}{m+1}(A)} \right)$$

.

Le right term is null almost everywhere with respect to the measure $\pi(dx) = dx$. We deduce that :

$$\int_0^1 P(x, A) dx = \int_0^1 \mathbb{1}_{x \notin I} \, \pi(A) dx = \pi(A) \int_0^1 \mathbb{1}_{x \notin I} \, dx = \pi(A)$$

The π is invariant with respect to the transition kernel P.

3. We have $x \notin I$, hence $P(x, \cdot) = \pi(\cdot)$:

$$Pf(x) = \int_0^1 f(y)P(x, dy) = \int_0^1 f(y)\pi(dy)$$

The function Pf si constant. We deduce that $x \notin I$, $P^nf(x) = \int_0^1 f(y)\pi(\mathrm{d}y)$ for all $n \geqslant 1$. Then $\lim_{x \to \infty} P^nf(x) = \int_0^1 f(y)\pi(\mathrm{d}y)$.

4. (a) We have $P\left(x, \frac{1}{m+1}\right) = 1 - x^2$. We show by induction the property $P^n\left(x, \frac{1}{m+n}\right) = \prod_{k=0}^{n-1} \left(1 - \frac{1}{(m+k)^2}\right)$. Let's show the induction step:

$$P^{n+1}\left(x,\frac{1}{m+n+1}\right) = \int_0^1 P\left(z,\frac{1}{m+n+1}\right) P^n\left(x,\mathrm{d}z\right) \text{ according to Chapman-Kolmogorov equation}$$

$$= P\left(\frac{1}{m+n},\frac{1}{m+n+1}\right) P^n\left(\frac{1}{m},\frac{1}{m+n}\right) \text{ car } P\left(z,\frac{1}{m+n+1}\right) = 0 \text{ if } z \neq \frac{1}{m+n}$$

$$= \prod_{k=0}^n \left(1 - \frac{1}{(m+k)^2}\right) \text{by induction hypothesis}$$

(b) It's easy to show that for $q \neq n-1$, $P^n\left(x, \frac{1}{m+1+q}\right) = 0$

$$P^{n}(x,A) = \sum_{q \in \mathbb{N}} P^{n}\left(x, \frac{1}{m+1+q}\right) = P^{n}\left(x, \frac{1}{m+n}\right) = \prod_{k=0}^{n-1} \left(1 - \frac{1}{(m+k)^{2}}\right)$$

We obtain:

$$P^n\left(x,\frac{1}{m+n}\right) = \prod_{k=0}^{n-1} \frac{m+k-1}{m+k} \prod_{k=0}^{n-1} \frac{m+k+1}{m+k} = \frac{m-1}{m+n-1} \frac{m+n}{m}$$

Then $\lim P^{n}(x, A) = \frac{m-1}{m} \neq 0 = \pi(A)$.

Exercice 3: Stochastic Gradient Learning in Neural Networks

1. We can notice that

$$R_n(w) = \frac{1}{n} \sum_{i=1}^n (y_i - w^T x_i)^2 = \mathbb{E}_{\mu_n} [(Y - w^T X)^2]$$

where $\mu_n = \frac{1}{n} \sum_{i=1}^n \delta_{(x_i, y_i)}$ is the empirical measure of (X, Y).

Algorithm 2 Stochastic Gradient Descent for minimizing empirical risk

Input: a sample $(x_i, y_i)_{1 \leqslant i \leqslant n}$ of size n

 $w \leftarrow w_0$, with random w_0 e.g $w_0 \sim \mathcal{N}(0, \sigma^2 I_2)$

 $k \leftarrow 1$

while not stopping criterion do

Sample $(x^k, y^k) \sim \mu_n$ $w \leftarrow w - \gamma_k \nabla_w F(x^k, y^k, w)$

 $k \leftarrow k + 1$

end while

Output: w

où
$$F(x,y,w)=(y-w^Tx)^2$$
 d'où $\nabla_w F(x,y,w)=-2(y-w^Tx)x,$ et $\gamma_k=\gamma/\sqrt{k}.$