M2 Mathématiques, Vision et Apprentissage
Computational statistics 2022 – 2023
Prof. Stéphanie Allassonnière **TP 1**

TP 1 : Reminder on Markov Chains – Stochastic gradient descent

Exercise 1 : Box-Muller and Marsaglia-Bray algorithm

Let R a random variable with Rayleigh distribution with parameter 1 and Θ with uniform distribution on $[0, 2\pi]$. We also assume that R and Θ are independent.

$$\forall r \in \mathbb{R}, \qquad f_R(r) = r \exp\left(-\frac{r^2}{2}\right) \mathbb{1}_{\mathbb{R}^+}(r)$$

1. Let X and Y such that

$$X = R\cos(\Theta) \qquad \text{and} \qquad Y = R\sin(\Theta)\,.$$

Prove that both X and Y have $\mathcal{N}(0,1)$ distribution and are independent.

2. Write an algorithm for sampling independent Gaussian distribution $\mathcal{N}(0,1)$.

Algorithm 1: Marsaglia-Bray algorithm

while $V_1^2 + V_2^2 > 1$ **do**
  Sample U_1, U_2 independant r.v. with distribution $\mathcal{U}([0,1])$;
  Set $V_1 = 2U_1 - 1$ and $V_2 = 2U_2 - 1$.
end
Set $S = \sqrt{-2\log(V_1^2 + V_2^2)}$;
Set $X = S\frac{V_1}{\sqrt{V_1^2+V_2^2}}$ and $Y = S\frac{V_2}{\sqrt{V_1^2+V_2^2}}$;
return (X, Y).

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3. Consider the algorithm given above.

a) What is the distribution of (V_1, V_2) at the end of the "while" loop ?

b) Set

$$T_1 = \frac{V_1}{\sqrt{V_1^2 + V_2^2}}, \qquad T_2 = \frac{V_2}{\sqrt{V_1^2 + V_2^2}} \qquad \text{and} \qquad V = V_1^2 + V_2^2\,.$$

Show that (T_1, T_2) and V are independent, $V \sim \mathcal{U}([0,1])$ and (T_1, T_2) has the same distribution as $(\cos(\Theta), \sin(\Theta))$ with $\Theta \sim \mathcal{U}([0, 2\pi])$.

c) What is the distribution of the output (X, Y) ?

d) What is the expected number of steps in the "while" loop ?

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Exercise 2 : Invariant distribution

We define a Markov chain $(X_n)_{n\geq 0}$ with values in $[0,1]$ as follows : given the current value X_n ($n \in \mathbb{N}$) of the chain,

- if $X_n = \dfrac{1}{m}$ (for some positive integer m), we let :

$$\begin{cases} X_{n+1} = \dfrac{1}{m+1} & \text{with probability } 1 - X_n^2 \\ X_{n+1} \sim \mathcal{U}([0,1]) & \text{with probability } X_n^2. \end{cases}$$

- if not, $X_{n+1} \sim \mathcal{U}([0,1])$.

1. Prove that the transition kernel of the chain $(X_n)_{n\geq 0}$ is given by :

$$P(x,A) = \begin{cases} x^2 \displaystyle\int_{A\cap[0,1]} dt + (1-x^2)\delta_{\frac{1}{m+1}}(A) & \text{if } x = \dfrac{1}{m} \\ \displaystyle\int_{A\cap[0,1]} dt & \text{otherwise.} \end{cases}$$

where δ_α is the Dirac measure at α.

2. Prove that the uniform distribution on $[0,1]$ is invariant for P. In the following, this invariant distribution will be denoted by π.

3. Let $x \notin \left\{\dfrac{1}{m},\, m \in \mathbb{N}^*\right\}$. Compute the value of $Pf(x) = \mathbb{E}[f(X_1) \mid X_0 = x]$, for a bounded measurable function f. Deduce $P^n f(x)$ for all $n \geqslant 1$. Compute $\lim\limits_{n\to+\infty} P^n f(x)$ in terms of $\int f(x)\pi(x)\,dx$.

4. Let $x = \dfrac{1}{m}$ with $m \geqslant 2$.

a) Let $n \in \mathbb{N}^*$. Compute $P^n\Big(x, \dfrac{1}{n+m}\Big)$ in terms of m and n.

b) Do we have $\lim\limits_{n\to+\infty} P^n(x,A) = \pi(A)$ when $A = \displaystyle\bigcup_{q\in\mathbb{N}} \left\{\frac{1}{m+1+q}\right\}$?

Exercise 3 : Stochastic Gradient Learning in Neural Networks, [Bot91, BCN16]

In the exercise, we consider the problem of classifying patterns x into two classes $y = \pm 1$. We assume that there is a relationship between a pattern and its class, embodied by some probability distribution $\mathbb{P}(x, y)$. If we know this distribution, we know the conditional probabilities $\mathbb{P}(y|x)$ as well, and we can solve immediately the problem using the Bayes decision rule. Learning means *"Acquiring enough knowledge about* $\mathbb{P}(x, y)$ *from the examples to solve the classification problem"*.

The statistical machine learning approach begins with the collection of a sizeable set of examples $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, where for each $i \in [\![1, n]\!]$ the vector x_i represents the *features* and the scalar y_i a *label* indicating whether x_i belongs ($y_i = 1$) or not ($y_i = -1$) to a particular class. With such a set of examples, one can construct a classification program, defined by a *prediction function* h, and measure its performance by counting how often the program prediction $h(x_i)$ differs from the correct prediction y_i. To avoid rote memorization, one should aim to find a prediction function that generalizes the concepts that may be learned from the examples. One way to achieve good generalized performance is to choose amongst a carefully selected class of prediction functions.

Thanks to such a high-dimensional sparse representation of documents, it has been deemed empirically sufficient to consider prediction functions of the form $h(x; w, \tau) = {}^t wx - \tau$. Here, ${}^t wx$ is a linear discriminant parameterized by $w \in \mathbb{R}^d$ and $\tau \in \mathbb{R}$ is a bias that provides a way to compromise between precision and recall, $\mathbb{P}[y = 1|h(x) = 1]$ and $\mathbb{P}[h(x) = 1|y = 1]$ respectively. The accuracy of the predictions could be determined by counting the number of times that $sign(h(x; w, \tau))$ matches the correct label, *i.e.*, 1 or -1. However, while such a prediction function may be appropriate for classifying new features, formulating an optimization problem around it to choose the parameters $(w; \tau)$ is impractical in large-scale settings due to the combinatorial structure introduced by the sign function, which is discontinuous. Instead, one typically employs a continuous approximation through a loss function that measures a cost for predicting h when the true label is y.

An **Adaline** (Widrow and Hoff, 1960) actually learns by (i) considering linear prediction function, $h(x, w) = {}^t wx$, and (ii) measuring the quality of the system through the mean squared error :

$$C_{Adaline}(w) = \int (y - h(x, w))^2 \, \mathrm{d}\mathbb{P}(x, y) = \int (y - {}^t wx)^2 \, \mathrm{d}\mathbb{P}(x, y) \, .$$

Learning consists of finding the parameter $w^\star$ that minimizes the above, or a more general, cost. This framework is the basis of classical statistical inference theory. Hundreds of practical algorithms have been derived.

In the following, we will denote by $z = (x, y)$ the observation and consider the cost or *expected risk* given a parameter vector w with respect to the probability $\mathbb{P}$

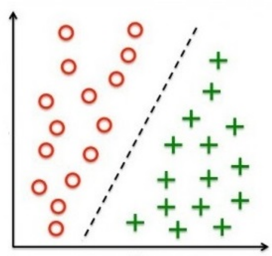
$$R(w) = \mathbb{E}[J(w, z)] = \int (y - {}^t wx)^2 \, \mathrm{d}\mathbb{P}(z) \, .$$

While it may be desirable to minimize the expected loss that would be incurred from *any* input-output pair, such a goal is untenable when one does not have complete information about $\mathbb{P}$. Thus, in practice, one seeks the solution of a problem that involves an estimate of the expected risk R. In supervised learning, one has access (either all-at-once or incrementally) to a set of $n \in N$ independently drawn input-output samples $\{z_i = (x_i, y_i)\}_{i=1}^n$ and one may define the *empirical risk* function $R_n \colon \mathbb{R}^d \to \mathbb{R}$ by

$$\boxed{R_n(w) = \frac{1}{n} \sum_{i=1}^{n} (y_i - {}^t wx_i)^2}$$

1. Describe the stochastic gradient descent algorithm for minimizing the empirical risk and implement it.

2. Sample a set of observations $\{z_i\}_{i=1}^n$ by generating a collection of random points x_i of $\mathbb{R}^2$, $\bar{w} \in \mathbb{R}^2$ seen as the normal vector of an hyperplane, a straight line here, and assigning the label y_i according to the side of the hyperplane the point x_i is.



3. Test the algorithm you wrote at the first question over these observations. What is the vector $w^\star$ estimated ? Is it far from $\bar{w}$?

4. Noise your observations $\{z_i\}_{i=1}^n$ with an additive Gaussian noise and perform the optimisation again. Compare with the result of question three.

5. Test the algorithm on the *Breast Cancer Wisconsin (Diagnostic) Data Set* [WSM95] : `http://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+%28Diagnostic%29`.

Références

[BCN16] Léon Bottou, Frank E. Curtis, and Jorge Nocedal. Optimization methods for large-scale machine learning. *eprint arXiv :1606.04838*, 2016.

[Bot91] Léon Bottou. Stochastic gradient learning in neural networks. In *Neuro-Nîmes 91*, 1991.

[WSM95] William H. Wolberg, W. Nick Street, and Olvi L. Mangasarian. UCI machine learning repository, 1995.