MATHÉMATIQUES
VISION
APPRENTISSAGE

Computational Statistics - TD1

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Exercise 1: Box-Muller and Marsaglia-Bray algorithm

1)

Let $h : \mathbb{R}^2 \to \mathbb{R}$ a measurable function:

$$\mathbb{E}(h(R\cos(\Theta), R\sin(\Theta))) = \int_{\mathbb{R}^+ \times [0,2\pi]} h(r\cos(\theta), r\sin(\theta)) \frac{1}{2\pi} r \exp\left(-\frac{r^2}{2}\right) dr d\theta$$

We perform the change of variable: $x = r\cos(\theta), y = r\sin(\theta)$

$$\det(J) = \begin{vmatrix} \cos(\theta) & -r\sin(\theta) \\ \sin(\theta) & r\cos(\theta) \end{vmatrix} = r$$

Hence:

$$\begin{aligned} \mathbb{E}(h(X,Y))) &= \frac{1}{2\pi} \int_{\mathbb{R}\times\mathbb{R}} h(x,y) \exp\left(-\frac{x^2+y^2}{2}\right) dx dy \\ &= \int_{\mathbb{R}\times\mathbb{R}} h(x,y) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right) dx dy \end{aligned}$$

So

$$\begin{aligned} f_{XY}(x,y) &= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right) \\ &= f_{X(x)} f_{Y(y)} \end{aligned}$$

$\boxed{\text{Hence, } X \text{ and } Y \text{ have } \mathcal{N}(0,1) \text{ distributions and are independent.}}$

2)

Given R with Rayleigh distribution of parameter 1 and $\Theta \sim \mathcal{U}[0, 2\pi]$, two independent variables, we're able to sample two random variables X and Y following a $\mathcal{N}(0,1)$ distribution.

Let $U \sim \mathcal{U}[0,1]$ and F_R the cdf of R.

- We know that $F_R^{-1}(U)$ has the same distribution as R. Indeed, let $T : [0,1] \mapsto \mathbb{R}$ a strictly monotone function such that $T(U)$ has the same distribution as R:

$$\begin{aligned} \forall r \in \mathbb{R}^+, F_R(r) &= \mathbb{P}(R \le r) && \text{Definition of a s cdf} \\ &= \mathbb{P}(T(U) \le r) && \text{Definition of } T \\ &= \mathbb{P}(U \le T^{-1}(r)) && T \text{ is strictly increasing, hence } T^{-1} \text{ as well} \\ &= T^{-1}(r) && \text{Because } U \text{ is uniform on } [0,1] \end{aligned}$$

And $F_R(r) = T^{-1}(r) \Leftrightarrow T(r) = F_R^{-1}(r)$.

- We compute F_R^{-1}:

$$\begin{aligned} F_R(r) &= \int_0^r r\exp\left(-\frac{r^2}{2}\right)dr \\ &= \left[-\exp\left(-\frac{r^2}{2}\right)\right]_0^r \\ &= 1-\exp\left(-\frac{r^2}{2}\right) \end{aligned}$$

So $F_R^{-1}(u) = \sqrt{-2\ln(1-u)} \qquad (u \in]0,1[)$

We finally deduce the algorithm:

sample $\Theta \sim \mathcal{U}[0, 2\pi]$
sample $U \sim \mathcal{U}]0, 1[$
$R \leftarrow \sqrt{-2\ln(1-U)}$
$X \leftarrow R\cos(\Theta)$
$Y \leftarrow R\sin(\Theta)$
return X, Y

3)

a)

V_1 and V_2 both have a uniform distribution on $[-1, 1]$ so **without** the `while` loop, $(V_1, V_2) \sim \mathcal{U}[-1, 1]^2$. The `while` loop ensures that $V_1^2 + V_2^2 \leq 1$, i.e that (V_1, V_2) lies in the unit disk. As any part of the disk is as likely to be sampled, we conclude that

after the `while` loop (V_1, V_2) has a uniform distribution on the unit disk.

b)

The `while` loop simulates independent Bernoulli trials of getting (V_1, V_2) such that $V_1^2 + V_2^2 \leq 1$. For one trial, the probability p of sampling inside the unit disk is the ratio between the area of the square $[-1, 1]^2$ and the area of the disk, hence $p = \frac{\pi}{4}$, hence the probability of sampling outside it is $q = 1 - p$.

Let T the random variable counting the number of trials needed to get one success. We denote by $V_i^{(k)}, i \in \{1, 2\}, k \in \mathbb{N}^*$ the k-th sampling of V_i:

$$\begin{aligned} \forall n \in \mathbb{N}^*, \mathbb{P}(T = n) &= \mathbb{P}\left(V_1^{(n)2} + V_2^{(n)2} > 1\right) \prod_{k=1}^{n-1} \mathbb{P}\left(V_1^{(k)2} + V_2^{(k)2} \leq 1\right) \\ &= q(1-q)^{n-1} \end{aligned}$$

So $T \sim \mathcal{G}(p)$, and the expected number of trials is $\mathbb{E}(T) = \frac{1}{q} = \frac{4}{4-\pi}$.

The expected number of steps is $\frac{4}{4-\pi}$

c)

The joint pdf of (V_1, V_2) after the `while` loop is given by:

$$f_{V_1,V_2}(v_1, v_2) = \frac{1}{\pi}\mathbb{1}_{\{v_{1^2}+v_{2^2}\leq 1\}}$$

We swith to polar coordinates for convenience: $V_1 = R\cos(\Theta), V_2 = R\sin(\Theta), R \in [0, 1], \Theta \in [0, 2\pi[$. So we can redefine $T_1 = \frac{V_1}{R} = \cos(\Theta)$ and $V = R^2$.

1. We first show that $V \sim \mathcal{U}[0,1]$:

$$F_V(v) = \mathbb{P}(V \leq v) = \mathbb{P}(R^2 \leq v) = \mathbb{P}\big(R \leq \sqrt{v}\big) = \int_0^{\sqrt{v}} \frac{1}{\pi} 2\pi r dr = \big(\sqrt{v}\big)^2 = v$$

thus: $f_V(v) = F_V{}'(v) = 1, \forall v \in [0,1]$

$\boxed{\text{Hence } V \text{ has a uniform distribution on } [0,1]}$

2. Since $\Theta \sim \mathcal{U}[0, 2\pi[$, its pdf is $f_\Theta = \frac{1}{2\pi}\mathbb{1}_{[0,2\pi[}$, continuous on $[0, 2\pi[$. As $T_1 = \cos\Theta$ (hence $\Theta = \arccos(T_1)$), we deduce that:

$$\begin{aligned}\forall t \in [-1,1], f_{T_1}(t) &= f_\Theta(\theta)\left|\frac{d\theta}{dt}\right| \\ &= \frac{1}{2\pi}\left|-\frac{1}{\sqrt{1-t^2}}\right| && \text{Derivative of arccos} \\ &= \frac{1}{2\pi}\frac{1}{\sqrt{1-t^2}}\end{aligned}$$

$\boxed{\text{So with } \Theta \sim \mathcal{U}[0,2\pi],\ T_1 \text{ has the same distribution as } \cos\Theta \text{ and its pdf is } t \mapsto \frac{1}{2\pi}\frac{1}{\sqrt{1-t^2}}.}$

3. R and Θ are independent random variables so any $f(R)$ and $g(\Theta)$ are also independent random variables, for any function f and g defined on $R(\Omega)$ and $\Theta(\Omega)$. By choosing $f : x \mapsto x^2$ and $g : x \mapsto \cos(x)$ we conclude that:

$\boxed{T_1 = g(\Theta) \text{ and } V = f(R) \text{ are independent.}}$

d)

Based on question 1. and 2., we can show that S has a Rayleigh distribution:

$$\begin{aligned}\forall s \geq 0, F_S(s) &= \mathbb{P}(S \leq s) && \text{Definition} \\ &= \mathbb{P}\Big(\sqrt{-2\log(V)} \leq s\Big) && \text{Using } \ V = V_1{}^2 + V_2{}^2 \\ &= \mathbb{P}\left(V \geq \exp\left(-\frac{s^2}{2}\right)\right) \\ &= 1 - \mathbb{P}\left(V \leq \exp\left(-\frac{s^2}{2}\right)\right) \\ &= 1 - \exp\left(-\frac{s^2}{2}\right) && \text{Because } \ V \sim \mathcal{U}[0,1]\end{aligned}$$

This shows that the cdf of S is the cdf of a Rayleigh distribution.

$\boxed{\text{So } S \text{ has a Rayleigh distribution.}}$

What's more we showed in question 3.c) that T_1 has the same distribution as $\cos(\Theta)$. We can show with the same reasoning that $\frac{V_2}{\sqrt{V_1{}^2+V_2{}^2}}$ has the same distribution as $\sin(\Theta)$.

With question 1. we conclude that both X and Y have a $\mathcal{N}(0,1)$ distribution.
Still with question 1., we know that X and Y are independent.

$\boxed{(X, X) \text{ follow a } \mathcal{N}(0, I_2) \text{ distribution.}}$

Exercise 2: Invariant distribution

1)

Let $n \geq 0$:

- We suppose that X_n can't be written as $\frac{1}{k}, (k \in \mathbb{N}^*)$
$$\begin{aligned}\mathbb{P}\left(X_{n+1} \in A | X_n \notin \left\{\tfrac{1}{k}, k \in \mathbb{N}^*\right\}\right) &= \int_A \mathbb{1}_{[0,1]}(t) dt \\ &= \int_{A \cap [0,1]} dt\end{aligned}$$
- We suppose that it exists a positive integer k such that $X_n = \frac{1}{k}$.
Let's define the random variable $Y_n \sim \mathcal{B}(X_n)$. We can reformulate the transition from X_n to X_{n+1} as follows:
$$\begin{cases} X_{n+1} = \frac{1}{k+1} & \text{if } \ Y_n = 0 \\ X_{n+1} \sim \mathcal{U}[0,1] & \text{if } \ Y_n = 1 \end{cases}$$

With the law of total probability we deduce that:

$$\begin{aligned}\mathbb{P}\left(X_{n+1} \in A | X_n = \frac{1}{k}\right) &= \mathbb{P}(Y_n = 0)\mathbb{P}\left(X_{n+1} | X_n = \frac{1}{k}, Y_n = 0\right) + \mathbb{P}(Y_n = 1)\mathbb{P}\left(X_{n+1} | X_n = \frac{1}{k}, Y_n = 1\right) \\ &= \left(1 - \frac{1}{k^2}\right)\delta_{\frac{1}{k}+1}(A) + \frac{1}{k^2}\int_{A \cap [0,1]} dt\end{aligned}$$

Hence we finally have:

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

2)

Let π the pdf of the uniform distribution on $[0, 1]$. We have $\pi(dx) = dx$:

- if $x \neq \frac{1}{k} (k \in \mathbb{N}^*)$:
$$\int_{[0,1]} P(x, A) dx = \int_{[0,1]} \int_{A \cap [0,1]} dt dx = \pi(A)$$
  - if $x = \frac{1}{k}, (k \in \mathbb{N}^*)$, the set $\left\{\frac{1}{k}, k \in \mathbb{N}^*\right\}$ is a countable set of real numbers, so it's Lebesgue measure is 0, so:
$$\int_{[0,1]} P(x, A) = \int_{[0,1]} \int_{A \cap [0,1]} dt dx = \pi(A)$$

We finally get the equality $\int_{[0,1]} P(x, A) \pi(dx) = \pi(A)$ for any measurable subset $A \subseteq [0, 1]$.

$\boxed{\pi \text{ is invariant to the transition kernel } P.}$

3)

Let $x \notin \left\{\frac{1}{k}, k \in \mathbb{N}^*\right\}$, we have:

$$
\begin{aligned}
Pf(x) &= \mathbb{E}[f(X_1)|X_0 = x] \\
&= \int f(t)P(x, dt) \qquad \text{Definition} \\
&= \int_{[0,1]} f(t)\pi(t)dt \qquad x \notin \left\{\frac{1}{k}, k \in \mathbb{N}^*\right\} \Rightarrow P(x, \cdot) = \pi(\cdot)
\end{aligned}
$$

Let $n \geq 1$:

$$
\begin{aligned}
P^n f(x) &= \mathbb{E}[f(X_n)|X_0 = x] \\
&= \mathbb{E}\left[f(X_n)|X_0 = x, X_1 \neq \frac{1}{k}, k \in \mathbb{N}^*\right]\mathbb{P}\left(X_1 \neq \frac{1}{k}, k \in \mathbb{N}^* \mid X_0 = x\right) \\
&+ \mathbb{E}\left[f(X_n)|X_0 = x, X_1 = \frac{1}{k}, k \in \mathbb{N}^*\right]\mathbb{P}\left(X_1 = \frac{1}{k}, k \in \mathbb{N}^* \mid X_0 = x\right) \text{ Law of total probilities}
\end{aligned}
$$

As $X_1 \mid X_0 = x \sim U[0, 1]$, we deduce that:

$$
\begin{cases}
\mathbb{P}\left(X_1 \neq \frac{1}{k}, k \in \mathbb{N}^* \mid X_0 = x\right) = 1 \\
\mathbb{P}\left(X_1 = \frac{1}{k}, k \in \mathbb{N}^* \mid X_0 = x\right) = 0
\end{cases}
$$

Because $\left\{\frac{1}{k}, k \in \mathbb{N}^*\right\}$ is countable, hence of null measure.

So

$$
\begin{aligned}
P^n f(x) &= \mathbb{E}\left[f(X_n) \mid X_0 = x, X_1 \neq \tfrac{1}{k}, k \in \mathbb{N}^*\right] \\
&= \mathbb{E}\left[f(X_n) \mid X_1 \neq \tfrac{1}{k}, k \in \mathbb{N}^*\right] \qquad \text{Markov property} \\
&= \mathbb{E}\left[\mathbb{E}[f(X_n) \mid X_{n-1}] \mid X_1 \neq \tfrac{1}{k}, k \in \mathbb{N}^*\right] \\
&= \mathbb{E}\left[f(X_{n-1}) \mid X_1 \neq \tfrac{1}{k}, k \in \mathbb{N}^*\right]
\end{aligned}
$$

By iteratively repeating the process we get:

$$
P^n f(x) = \mathbb{E}[f(X_1) \mid X_0 = x] = \int_{[0,1]} f(t)\pi(t)dt
$$

We conclude that

$$
\boxed{\lim_{n \to +\infty} P^n f(x) = \int_{[0,1]} f(t)\pi(t)dt}
$$

4)

Let $x = \frac{1}{k}$, $k \geq 2$:

a)

Now we have $P(x, A) = x^2 \int_{A \cap [0,1]} dt + (1 - x^2)\delta_{\frac{1}{k+1}}(A)$.

If $x = \frac{1}{k}$, the chain can reach:

$$
\begin{cases}
\frac{1}{k+1} \text{ with a probability } 1 - \frac{1}{k^2} \\
\text{be uniformly distributed on } [0, 1] \text{ with probability } \frac{1}{k^2}
\end{cases}
$$

So to reach $\frac{1}{k+n}$ after n steps, the chain should always reach $\frac{1}{k+i}$, $(0 \leq i \leq n)$, as it's very unlikely to reach $\frac{1}{k+n}$ if it's resampled at least once uniformly on $[0,1]$.
Hence we expect the probability to reach $\frac{1}{k+n}$ starting form $\frac{1}{k}$ after n steps with a probability $\prod_{i=1}^{n-1}\left(1-\frac{1}{(k+i)^2}\right)$

So we show by induction on $n \in \mathbb{N}^*$, $\mathcal{P}_n : P^n\left(\frac{1}{k}, \frac{1}{k+n}\right) = \prod_{i=0}^{n-1}\left(1-\frac{1}{(k+i)^2}\right)$

- For $n = 1$ we have $P\left(\frac{1}{k}, \frac{1}{k+1}\right) = \left(1-\frac{1}{k^2}\right)$ by definition of the transition kernel.
- Let $n \in \mathbb{N}^*$, we suppose that we have $\mathcal{P}_n$.

$$\begin{aligned}
P^{n+1}\left(\frac{1}{k}, \frac{1}{k+n+1}\right) &= P\left(P^n\left(\frac{1}{k}, \frac{1}{n+k+1}\right)\right) \\
&= \int_{[0,1]} P\left(t, \frac{1}{k+n+1}\right) P^n\left(\frac{1}{k}, dt\right) \\
&= P\left(\frac{1}{n+k}, \frac{1}{n+k+1}\right) P^n\left(\frac{1}{k}, \frac{1}{n+k}\right) \qquad P\left(t, \frac{1}{n+k+1}\right) = 0 \text{ for } t \neq \frac{1}{n+k} \\
&= \left(1-\frac{1}{(k+n)^2}\right) \prod_{i=1}^{n-1}\left(1-\frac{1}{(k+i)^2}\right) \qquad \text{As we have } \mathcal{P}_n
\end{aligned}$$

So

$$\boxed{P^n\left(\frac{1}{k}, \frac{1}{k+n}\right) = \prod_{i=1}^{n-1}\left(1-\frac{1}{(k+i)^2}\right)}$$

b)
Let $A = \bigcup_{q \in \mathbb{N}} \left\{\frac{1}{k+1+q}\right\}$. We have:
- $P^n(x, A) \neq 0 \Leftrightarrow \delta_{\frac{1}{k+n}}(A) \neq 0 \Leftrightarrow q = n-1$
- $\pi(A) = 0$ because a is a countable set, hence for null Lebesgue measure.

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

$$\begin{aligned}
\prod_{i=1}^{n-1}\left(1-\frac{1}{(k+i)^2}\right) &= \prod_{i=1}^{n-1}\left(1-\frac{1}{k+i}\right)\prod_{i=1}^{n-1}\left(1+\frac{1}{k+i}\right) \\
&= \prod_{i=1}^{n-1}\left(\frac{k+i-1}{k+i}\right)\prod_{i=1}^{n-1}\left(\frac{k+i+1}{k+i}\right) \\
&= \frac{k}{k+n-1} \times \frac{k+n}{k+1} \qquad \text{Telescopic product} \\
&= \frac{k}{k+1} \times \frac{k+n}{k+n-1} \underset{n \to +\infty}{\longrightarrow} \frac{k}{k+1}
\end{aligned}$$

$$\boxed{\lim_{n \to +\infty} P^n\left(\frac{1}{k}, A\right) = \frac{k}{k+1} \neq 0 = \pi(A)}$$

Exercise 3: Stochastic Gradient Learning in Neural Networks

1)

Input:
$\left\{(x_i, y_i)_{i \in [\![1,n]\!]}\right\}$ a set of input-output samples ($n \in \mathbb{N}$)
$(\eta_k)_{k \in \mathbb{N}}$ a sequence of learning rates
ε a tolerance

$w \leftarrow w_0$
$k \leftarrow 1$
while not stopping criterion :
  sample $\left(x_{i_k}, y_{i_k}\right) \in \left\{(x_i, y_i)_{i \in [\![1,n]\!]}\right\}$
  $w \leftarrow w + \eta_k \nabla_w R\left(w_k, x_{i_k}, y_{i_k}\right)$
  $k \leftarrow k + 1$
output w

Where:

- $\nabla_w R\left(w_k, x_{i_k}, y_{i_k}\right) = -2\left(y_{i_k} - w^T x_{i_k}\right) x_{i_k}$
- $\eta_k = \eta_0 d^{\lfloor \frac{k+1}{r} \rfloor}, (\eta_0 < 1)$
  Defining the learning rate series that way, it's updated every r steps of the descent, and decreased by a ratio d. There are many other ways to define this sequence, but this one is intuitive.

  Here is an implementation of the algorithm that can be found in this notebook:

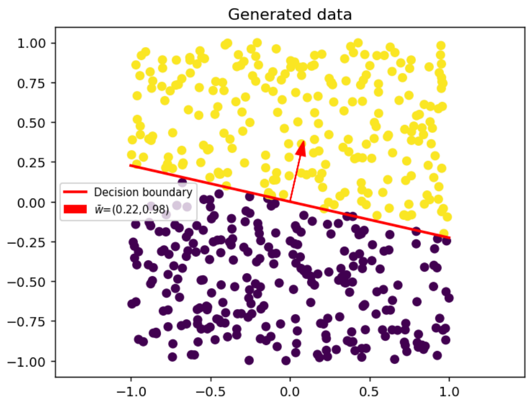
```
def SGD(X, y, max_iter, init_lr, d=0.7, r=10):
    """
    init_lr: initial learning rate
    d: how much the learning rate should change at each drop
    r: drop rate (how often the rate should be dropped)
    """

    w = np.random.randn(X.shape[1])
    losses = []
    accuracies = []

    for i in range(max_iter):
        lr = init_lr * d**np.floor((i+1) / r)
        k = np.random.randint(0, len(y))
        x_k, y_k = X[k,:], y[k]

        # Weights update
        w += lr * 2 * (y_k-w @ x_k.T) * x_k
        w /= norm(w) # set norm to 1

        y_pred = predict(X, w)
        accuracies.append(accuracy(y_pred, y))
        loss = np.mean((y - w @ X.T)**2)
        losses.append(loss)

    return w, losses, accuracies
```

Note about the code: The accuracy function is coded in the notebook and implements the following formula:

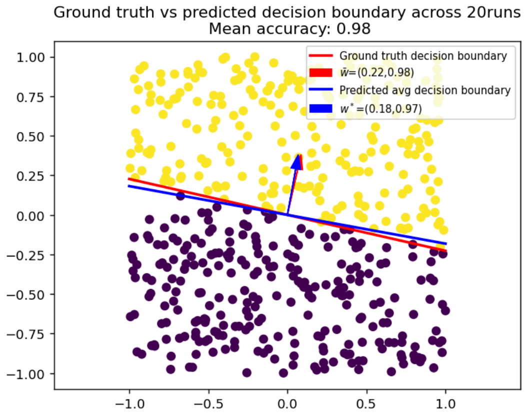
$$\text{Accuracy}(\hat{y}, y) = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i| \qquad (\hat{y}, y) \in \mathbb{R}^n$$

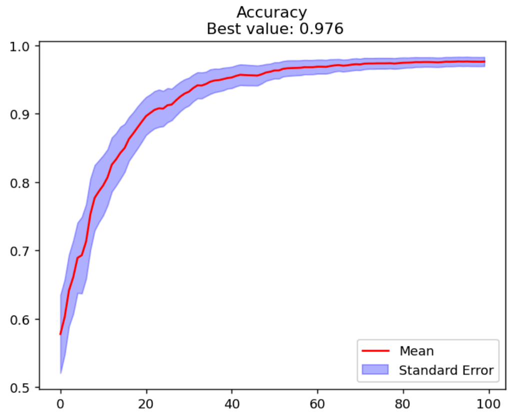
2)

The code used to generate the following figures can be found on this notebook.



3)





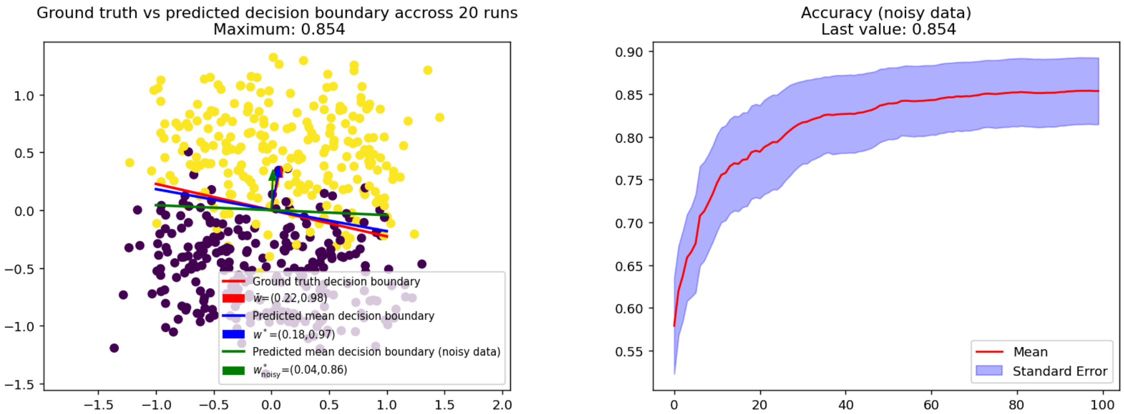
The training process was performed with the following hyper-parameters on `n = 500` data points. To be able to estimate the standard error, thus evaluating the robustness of the model, the training is repeated `n_runs = 20` times. The red curve on the accuracy plot correspond to the mean curve cross the `n_runs` attempts. Finally we use the classical standard error estimator $\sigma_{\text{std}} = \frac{\hat{\sigma}}{\sqrt{n_{\text{runs}}}}$.

Here are specified the hyper-parameters used to generate the plots:

- `init_lr =  0.1`
- `max_iter = 100`
- `n_runs =  20`

We get a boundary close to the ground truth with a low standard error, as illustrated in the accuracy curve.

4)



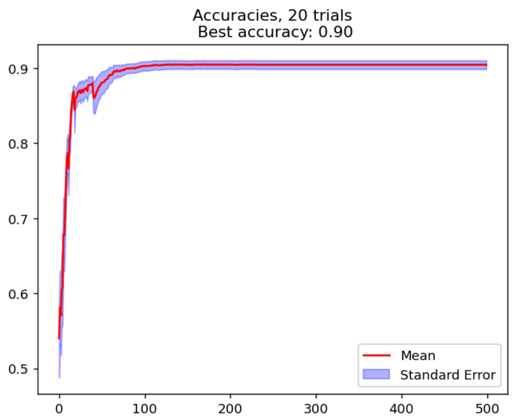
Noisy data was generated by adding a Gaussian noise of mean 0 and variance 0.04.

We notice that the decision boundary predicted on noisy is farther from the ground-truth than the one predicted on not noisy data. In addition, the accuracy curve shows that the standard error is larger than for the non-noised version of the dataset.

5)

Implementation details for the Breast Cancer Wisconsin dataset

- 30% of the dataset is used as a test set
- The training set is standardized so that we don't have to fit a bias
- The test set is standardized using the mean and the variance computed on the training set
- `lr_init = 0.008`
- `max_iter = 500`
- `n_runs = 20`



We get an accuracy of 0.89 ± 0.01 on the test set.