ML3 - Practical Class n°1

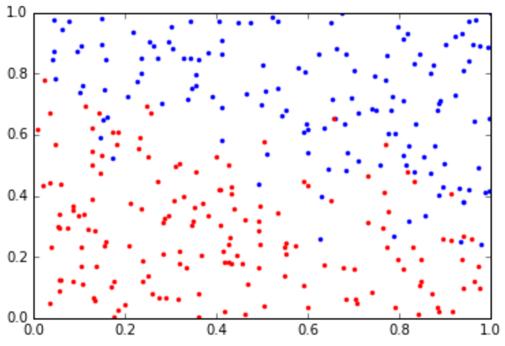
This practical class contains a reminder on logistic regression and basic gradient descent techniques.

Exercise n°1 : Logistic regression by gradient descent

In this exercise, we will use logistic regression to solve in binary classification task. The parameters of the model will be learned by batch gradient descent and its stochastic version.

Questions :

1. Create a `datagen` function allowing to create a dataset with inter-class overlapping.
   To that end, draw inputs uniformly in the unit square. This implies that inputs $\mathbf{x} \in \mathbb{R}^2$ and $0 \leq x_1, x_2 \leq 1$.
   To create an overlap, the class label of each generated input must be chosen as follows :
   — determine the signed distance[1] D between the generated input and the line whose equation is $x_2 = -0.5x_1 + 0.75$,
   — if $D > 0$, assign class label 1, otherwise assign class label 0,
   — compute $r = e^{-\frac{D^2}{2\sigma^2}}$ with $\sigma = 0.05$,
   — draw a sample $Z \sim \text{Ber}\left(\frac{r}{2}\right)$,
   — if $z = 1$ then, change the class label.
   Calling this function to generate a dataset with $n = 300$ points should give something like this :



2. Create a python variable `X_plus` by concatenating `X` with a line of 1 as :

$$\mathbf{X}_+ = \begin{pmatrix} \begin{bmatrix} \mathbf{x}^{(1)} \end{bmatrix} & \cdots & \begin{bmatrix} \mathbf{x}^{(n)} \end{bmatrix} \\ 1 & \cdots & 1 \end{pmatrix}. \quad (1)$$

3. Let us start training a logistic regression by gradient descent. Logistic regression is meant to find a separating hyperplan (a line in our case). This hyperplan in question is parametrized by a normal vector $\mathbf{w}$ and a constant b, called *intercept*. To have more compact notations, let us introduce the following

1. See section 4.1.1 p. 181 of [Bishop].

vector parameters

$$\boldsymbol{\theta} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \\ b \end{bmatrix}. \tag{2}$$

The classical gradient descent, by opposition to the stochastic one, is called *batch* descent meaning that all data is used to compute one gradient vector. Subtracting this gradient to the vector of parameters allows to decrease the NLL / train loss.

```
Initialize $\boldsymbol{\theta}_0$ and $\eta$.
while not converged do
    Compute predictions : $\mathbf{pred} \leftarrow \text{sgm}\left(\mathbf{X}_+^T.\boldsymbol{\theta}_t\right)$.
    Compute signed errors : $\mathbf{err} \leftarrow \mathbf{pred} - \mathbf{y}$.
    Compute gradient : $\mathbf{g} \leftarrow \mathbf{X}_+ \cdot \mathbf{err}$
    Update parameters : $\boldsymbol{\theta}_{t+1} \longleftarrow \boldsymbol{\theta}_t - \eta \times \mathbf{g}$.
end while
```

For the time being, the *learning rate* η has a constant value.

Implement this procedure in python so that it returns the whole history of parameter vectors $\boldsymbol{\theta}$ across iterations. This history is stored in a 2D `numpy array` called `thetas` whose size is $3\times$ the number of iterations.

4. Try your implementation with $\eta = 0.02$ and $\eta = 0.1$. Visualize the results thanks to the following code :

```
from mpl_toolkits.mplot3d import Axes3D
fig = plt.figure()
ax = fig.gca(projection='3d')
ax.plot(thetas[0],thetas[1],thetas[2],'-o')
plt.draw()
```

5. Let us go stochastic. The procedure becomes :

```
Initialize $\boldsymbol{\theta}_0$ et $\eta$.
while not converged do
    Draw a permutation $\sigma$ at random.
    Use this permutation on examples : $\mathbf{X}_+ \leftarrow \sigma\left(\mathbf{X}_+\right)$
    Use the same permutation on class labels : $y \leftarrow \sigma\left(y\right)$
    for  $i$ from 1 to $n$ do
        Compute prediction for the $i^{\text{th}}$ example : pred $\leftarrow$ sgm $\left({\mathbf{x}_+^{(i)}}^T.\boldsymbol{\theta}_t\right)$.
        Compute its signed error : $err \leftarrow \text{pred} - y^{(i)}$.
        Compute its gradient : $\mathbf{g} \leftarrow \mathbf{x}_+^{(i)} \times err$
        Update parameters : $\boldsymbol{\theta}_{t+1} \longleftarrow \boldsymbol{\theta}_t - \eta \times \mathbf{g}$.
    end for
end while
```

Implement this procedure in python and store the history of values of $\boldsymbol{\theta}$ and the number of « epochs[2] ».

Indication :For the permutation, you may use `numpy.random.permutation`.

6. Try your implementation with $\eta = 1.5$ Visualize the trajectory of $\boldsymbol{\theta}$ with the same 3D plot as before.
7. Compare the results by displaying the learned separating lines on the scatter-plot of the data. Also compare the number of « epochs » in SGD to the number of iterations of the batch method.
8. Propose a modification (few lines of code) to the SGD algorithm so that gradients are computed from a mini-batch of 10 examples.

Proof of gradient formula for log. reg.

Recall from the class that the logitic regression loss for example $\mathbf{x}^{(i)}$ is given by

$$\ell_i = -y^{(i)} \log \text{sgm}\left(\boldsymbol{\theta}^T \cdot \mathbf{x}_+^{(i)}\right) - (1 - y^{(i)}) \log\left(1 - \text{sgm}\left(\boldsymbol{\theta}^T \cdot \mathbf{x}_+^{(i)}\right)\right).$$

2. The number of times each data point was used, i.e. the number of times the for loop is executed.

Let us differentiate ℓ_i w.r.t. the vector $\boldsymbol{\theta}$:

$$\frac{d\ell_i}{d\boldsymbol{\theta}} = -y^{(i)}\frac{d}{d\boldsymbol{\theta}}\log\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right) - (1-y^{(i)})\frac{d}{d\boldsymbol{\theta}}\log\left(1-\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)\right), \tag{3}$$

$$= -y^{(i)}\frac{d}{d\boldsymbol{\theta}}\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)\frac{1}{\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)} - (1-y^{(i)})\frac{d}{d\boldsymbol{\theta}}\left(1-\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)\right)\frac{1}{1-\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)}. \tag{4}$$

Given that $\mathrm{sgm}' = \mathrm{sgm}\,(1-\mathrm{sgm})$, we have

$$\frac{d\ell_i}{d\boldsymbol{\theta}} = -y^{(i)}\underbrace{\frac{d}{d\boldsymbol{\theta}}\left\{\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right\}}_{=\mathbf{x}_+^{(i)}}\frac{\mathrm{sgm}'\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)}{\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)} - (1-y^{(i)})\frac{d}{d\boldsymbol{\theta}}\left\{\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right\}\frac{-\mathrm{sgm}'\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)}{1-\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)}, \tag{5}$$

$$= \mathbf{x}_+^{(i)}\left[-y^{(i)}\left(1-\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)\right) + (1-y^{(i)})\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)\right], \tag{6}$$

$$= \mathbf{x}_+^{(i)}\left[\underbrace{\mathrm{sgm}\left(\boldsymbol{\theta}^T\cdot\mathbf{x}_+^{(i)}\right)}_{\text{pred}} - y^{(i)}\right]. \tag{7}$$

Finally,

$$\frac{d\mathrm{NLL}}{d\boldsymbol{\theta}} = \sum_i \frac{d\ell_i}{d\boldsymbol{\theta}}, \tag{8}$$

$$= \mathbf{X}_+\cdot\mathbf{err}. \tag{9}$$