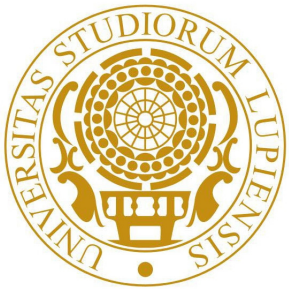
UNIVERSITÀ DEL SALENTO



Facoltà di Ingegneria

Corso di Laurea Magistrale in Computer Engineering

Advanced Control Techniques Project

Multinomial Logistic Regression for a Supervised Learning problem

Professor: **Giuseppe Notarstefano**

Students: **Alfarano Gianluca,**
Basile Davide,
Capoccia Leonardo,
Larini Ludovico

Academic year 2017/2018

Abstract

In this report, it will be shown how to solve a Multinomial Logistic Regression (also known as *Softmax Regression*) using a distributed method. The sub-gradient method has been used to distribute calculations among a configurable number of agents. A portion of the dataset is given to each agent and used to minimize a cost function related to the portion of the dataset in its possession. A Python3 program has been written supported by several libraries. The most important library is MPI4py which provides implementation of the MPI specifics. MPI is a communication protocol between nodes that executes the same program in parallel. We compared the results obtained through this program with MATLAB script which executes all operation with a centralized architecture (meaning that all operations are executed by a single agent).
Several graphs are plotted in order to see the graph of communicating agents, how the consensus is reached and how the cost diminishes to a minimum.

Contents

List of Figures

Introduction

Motivations

In the past there was a single *Mainframe* that executed all digital computations. Years after, with the creation of the Personal Computer, more people could execute the same operations in private. Today's *Microcontrollers* allow to make smart all the of devices. More algorithms have been created to connect these devices to distribute.
In general, this approach is useful because it allows cooperation between agents, to reach a common goal. In this case, the ability to split the workload in to several agents guarantees faster execution times. The Multinomial Logistic Regression generalizes the logistic regression for a multiclass problem, with more than two possible discrete outcomes, where each observation has several features.

Contributions

This work implements a scenario in which there are some agents that estimate a cost function using their own information and those of other agents; they use a *Distributed Sub-gradient Method* to update their own estimate and, in particular, they resolve a *Multinomial Logistic Regression* problem.

The first step was to create a MATLAB script that solves a quadratic optimization problem using a gradient method. In this script it has been *simulated* a distributed approach in order to test the effectiveness of the method saw in Distributed Subgradient Methods for Multi-Agent Optimization [1]. MATLAB was only used in the prototype phase, because it doesn't allow real parallel computations. After the confirmation that the approach was working, it started the implementation of the algorithm in Python3 using the Message Passing Interface.
The quadratic form used was

$$x^T Q x + r^T x \tag{I}$$

.
This form was used only to test the convergence of the method.

After established that, considering that the Supervised Learning problem known as Multinomial Logistic Regression gives as output a probability value for every considered class, it was necessary to implement the softmax function.

$$g_i(\theta) := \sum_{k=1}^{K} 1\{y^{(i)} = e_k\} \log\left(\frac{exp(\theta^{(k)^\top} x^{(i)})}{\sum_{k=1}^{K} exp(\theta^{(j)^\top} x)}\right) \tag{II}$$

[3].
The formula saw in 1.7 was minimized in a centralized setup using MATLAB, and the result was compared to the one of the Python distributed program.
It was seen that the algorithm was converging, several tests were executed to find the optimal values for the step-size.
The present work is divided into two chapters. In Chapter 1, it is introduced the theory behind the problem and it is visualized and commented the implementation code. In Chapter 2 there are the results of simulations with some considerations.

Chapter 1

Problem and its implementation

1.1 Theory of the problem

1.1.1 Distributed Subgradient Methods for Multi-Agent Optimization

In this problem there are m agents that cooperatively minimize a common additive cost. The general optimization problem is:

$$min \quad \sum_{i=1}^{m} f_i(x) \qquad subject\ to \quad x \in \mathbb{R}^n, \tag{1.1}$$

where $f_i : \mathbb{R}^n \longrightarrow \mathbb{R}$ is the cost function of agent i, known only by the agent i, and $x \in \mathbb{R}^{\times}$ is the decision vector. It is assumed that:

- the cost function is convex;
- the agents are distributed over a time-varying topology;
- the graph (V, E_∞) is connected, where E_∞ is the set of edges (j, i) representing agent pairs communicating directly an indefinite number of times;
- there is not communication delay.

Every agent i generates and maintains an estimate of the optimal decision vector based on information concerning its own cost function and exchanges this estimate with its neighbours at discrete times $t_0, t_1, t_2, ...$ A weights matrix is associated to the communication graph, and its elements are defined as follows:

$$\begin{cases} > 0, & \text{if } (i,j) \in E(k) \\ 0, & \text{otherwise} \end{cases}$$

Each agent j that receives an information by a neighbour agent i weights this information by multiplying it by $a_i^j(k) \in \mathbb{R}$. Then the update of the estimate of the optimal solution is update according to:

$$x^i(k+1) = \sum_{j=1}^{m} a_j^i(k)\, x^i(k) - a^i(k)\, d_i(k) \tag{1.2}$$

where $\alpha^i(k) > 0$ is the step-size used by agent i and the vector $d_i(k)$ is a sub-gradient of objective function $f_i(x)$ calculated at $x = x^i(k)$. [1]

1.1.2 Multinomial Logistic Regression

The problem to be solved is a Supervised Learning problem called Multinomial Logistic Regression, also known as Softmax Regression, and it generalizes the more common Logistic Regression. The difference between them is that in the former there are several classes to be considered, in the latter, there are only two classes (or equivalently a binary class).
The problem to be solved is to find a set of coefficients based on a given dataset to predict the belonging class for an unseen set of features, while minimizing a cost function. The dataset is composed of N labelled examples $\{(x^{(1)}, y^{(1)}), ..., (x^{(N)}, y^{(N)})\}$. Each $x^{(i)} \in R^{d_x}$ for $i = 1, ..., N$ is composed of some features which represent the value upon which we base the estimation of the belonging class, while $y^{(i)} \in R^{d_y}$ is the belonging class for the *i-th* example, and can be a values in $\{1, ..., K\}$.

Given a single training example $(x^{(i)}, y^{(i)})$, the definition of the cost function is:

$$f_i(\omega) := \left|\left| h_\omega\left(x^{(i)}\right) - y^{(i)} \right|\right|^2 \tag{1.3}$$

where the $\omega \in R^{d_x}$ are the weights of the hypothesis function h_ω. The overall cost function can be defined as:

$$f(\omega) := \sum_{i=1}^{N} f_i(\omega) \tag{1.4}$$

We solve the problem by finding the solution of the following optimization problem:

$$\omega^* := \arg\min_{\omega} f(\omega) \tag{1.5}$$

In the Multinomial Logistic Regression, a common choice for the hypothesis function is the following:

$$h_\theta = \frac{1}{\sum_{j=1}^{K} exp\left(\theta^{(j)\top} x\right)} \begin{bmatrix} exp\left(\theta^{(1)\top} x\right) \\ \vdots \\ exp\left(\theta^{(K)\top} x\right) \end{bmatrix} \tag{1.6}$$

where the weights $\omega = \theta = (\theta^{(1)}, ..., \theta^{(K)}) \in R^{d_x}$.
Using this function, the solution of the problem is given by finding:

$$\theta^* = \arg\min_{\theta} - \sum_{i=1}^{N} g_i(\theta) \tag{1.7}$$

with

$$g_i(\theta) := \sum_{k=1}^{K} 1\{y^{(i)} = e_k\} \log \left(\frac{exp(\theta^{(k)^\top} x^{(i)})}{\sum_{k=1}^{K} exp(\theta^{(j)^\top} x)} \right) \tag{1.8}$$

where $\mathbf{1\{\cdot\}}$ being the *indicator function*. [2]

1.1.3 Pseudocode

Algorithm 1

Stop Rules:
$||\theta_{k+1} - \theta_k|| \leq \varepsilon$ $\quad$ ε fixed
Number of maximum iterations reached
Start:
Fix initial conditions for each node $\theta_i(0) = [0 \quad ... \quad 0]^T$
Define the Adjacency Matrix, Weights Matrix, $\alpha^i = \alpha$ constant for each iteration
while No stop rule is true, each node i does: **do**
    calculate ∇f_i
    for each neighbour j **do**
        $\theta_i(k+1) = \theta_i(k+1) + a_j^i(k)\theta^j(k)$
    end for
    $\theta_i(k+1) = \theta_i(k+1) - \alpha \nabla f_i$
end while
Result:
Each node i should converge to θ^*
The minimum of function is $\sum_{i=1}^{m} f_i(x^*)$

1.2 Code Implementation

Here is defined and explained the Python imlementation that solves the problem. The solution has been implemented using: *numpy* library which computes all vector and matrix operation such as transposition, product, division, summation; *networkx* which creates and manages adjacency matrices for all agent; *matplotlib* that plots the results with data from the test and training phases. At first, the code checks if all the paramethers are valid,

then it starts to create the environment, the adjacency matrix and it initializes the local variables where the data will be saved. The weights depend on how many in-neighbours each agent has. The number of in-neighbours for each agent can be passed as a paramether at launch, by specifying it with -k .

The adjacency matrix is created by the *createAdjM* function. It makes a communication graph using world_d as number of mpi agents, n_edges (setted by default as 1), phi that is simply a phase inserted into graph which just shift the connection, by default is 0 (TODO: la parte di phi non mi convince). The first for cycle sets the number of agents that the system has, then edges are computed as follows:

- The sum j + k + phi + 1 means the position of edge in the graph where item j is the current row, k is the count of agent that the agent j will send a message, phi is the phase and just shift the agent that j will send a message and the "+1"
- The instruction $if\ e >= world\_d$ checks if the sum is over the number of agents and if is true just subtracts this one
- Instead $if\ e == j$ removes the hypothetical unnecessary self loop.

Loss softmax function,*loss_softmax* gets as parameter the current state(*all_theta*), the cardinality of iris set (*category_count*), the agent dataset (*personal_dataset*) and a *CONSTANT_TO_SUBTRACT*, a constant to prevent overflow.
The algorithm wants to calculate the $\sum_{i=0}^{number\_of\_agents} f_i(x)$ and this function calculate the agent i $f(x)$. This is done as follows: for every row in the personal dataset, the algorithm computes the denominator that is the sum over all exponential. Then it computes, category by category, row by row, the logarithm of ratio between the sum previously calculated and the exponential of the row. After that, there's the summation of all calculated elements.

```
1  def loss_softmax(all_theta, category_count, personal_dataset,
       CONSTANT_TO_SUBTRACT):
2      the_sum = 0
3
4      for index in range(0, len(personal_dataset)):
5          denominator = 0
6
7          for theta in all_theta:
8              denominator = denominator + np.exp(np.dot(theta,
                   personal_dataset[index][0:4]) - CONSTANT_TO_SUBTRACT)
9
10         for category in range(0, category_count):
11
12             if category == personal_dataset[index][4]:
13                 _exp = np.exp(np.dot(all_theta[category],
                       personal_dataset[index][:4]) -
                       CONSTANT_TO_SUBTRACT)
```

```
14                  _log = np.log(np.divide(_exp, denominator))
15                  the_sum = the_sum - _log
16
17      return the_sum
```

In the function *gradient_softmax* there is implemented the gradient of softmax equation. It is calculated similarly as the function mentioned before: calculate in a first time the sum of all exponential theta and then sum for each coefficient, subtract from one that coefficient and finally subtract the dataset normalized with that to the respective theta.

```
1  def gradient_softmax(all_theta, category_count):
2
3      thetas = np.zeros(dimensions)
4
5      for index in range(0, len(personal_dataset)):
6          denominator = 0
7
8          for theta in all_theta:
9              denominator = denominator + np.exp(np.dot(theta,
                   personal_dataset[index][:4]) - CONSTANT_TO_SUBTRACT)
10
11         for category in range(0, category_count):
12             coeff = 0
13
14             if category == personal_dataset[index][4]:
15                 coeff = 1
16
17             _exp = np.exp(np.dot(all_theta[category], personal_dataset
                   [index][:4]) - CONSTANT_TO_SUBTRACT)
18             coeff = coeff - np.divide(_exp, denominator)
19             thetas[category] = thetas[category] - ((1/len(
                   personal_dataset)) * np.multiply(personal_dataset[
                   index][:4], coeff))
20
21     return thetas
```

1.2.1 working.py

In this file is implemented the main algorithm where the loss function is minimized and the consensus is reached.

The complete iris training set is loaded, and some environment variables are setted like the number of agents. Then the dataset is splitted in equal parts to all agents and each one gets its own piece and it prints how many row it has.

Every agent creates the same communication directed graph with number of agents and number of in connection. Then state and loss variable are created, setted to 0 of *MAX_ITERATIONS* size. In order to get weight the messages, all in-neighbours are found and the variable *weight* is setted as the average. If the function name inserted is "quadratic" Q and r variables

are created randomly. *epsilon_reached* and *buff* are epsilon checker variable that say to agent when they have to exit from the loop (if epsilon is reached).

This *for* cycle calculates the consensus. For every *iters*, is calculated the new "diminishing" alpha; message(s) are sent and received, then local variable are weighted. In order to solve consensus to desiderated function, the three implemented ones are inserted into an *if* clause, and the right function is called. After that, the calculated gradient is multiplied by alpha and then new state is calculated. Then *lossfunction* is called and if $\|XX[tt] - XX[tt-1]\| \leq epsilon$ then buff is true and rank 0 check if all agent has reached the epsilon condition; if true it sends a broadcast message with a *true* value to say to all that the cycle is done.

```
for tt in range(1, MAX_ITERATIONS - 1):

    if alpha_type == "diminishing":
        alpha = psi_coefficient * (1 / tt) ** alpha_coefficient
    else:
        alpha = alpha_coefficient

    # Update with my previous state
    u_i = np.multiply(XX[tt - 1], weight)

    # Send the state to neighbors
    for node in adj.successors(rank):
        world.send(XX[tt - 1], dest=node)

    # Update with state of all nodes before me
    for node in adj.predecessors(rank):
        u_i = u_i + world.recv(source=node) * weight

    # Go in the opposite direction with respect to the gradient
    gradient = 0

    if function_name == "softmax":
        gradient = func.gradient_softmax(XX[tt - 1], category_n,
            dimensions, personal_dataset, CONSTANT_TO_SUBTRACT)

    elif function_name == "quadratic":
        gradient = func.gradient_quadratic(XX[tt - 1], category_n,
            dimensions, personal_dataset, Q, r)

    elif function_name == "exponential":
        gradient = func.gradient_exponential(XX[tt - 1], category_n,
            dimensions, personal_dataset, CONSTANT_TO_SUBTRACT)

    #print(gradient)

    grad = np.multiply(alpha, gradient)

    for i in range(0, dimensions[0]):
        u_i[i] = np.subtract(u_i[i], grad[i])

    # Store  my new state
    XX[tt] = u_i

    if function_name == "softmax":
        losses[tt] = func.loss_softmax(XX[tt], category_n,
            personal_dataset, CONSTANT_TO_SUBTRACT)
```

```
43
44      elif function_name == "quadratic":
45          losses[tt] = func.loss_quadratic(XX[tt], category_n,
                dimensions, personal_dataset, Q, r)
46
47      elif function_name == "exponential":
48          losses[tt] = func.loss_exponential(XX[tt - 1], category_n,
                dimensions, personal_dataset, CONSTANT_TO_SUBTRACT)
49
50      # Checking epsilon reached condition
51      if np.linalg.norm(np.subtract(XX[tt], XX[tt - 1])) < epsilon:
52          buff = True
53
54      # Rank 0 get all epsilon and check if all reached it
55      buffer = world.gather(buff, root=0)
56
57      # If true it set epsilon reached
58      if rank == 0:
59          if False not in buffer:
60              epsilon_reached = True
61
62      # Send epsilon reached to all agents
63      epsilon_reached = world.bcast(epsilon_reached, root=0)
64
65      # Check if all agent have reached epsilon condition and then exit
            from loop
66      if epsilon_reached:
67          if rank == 0:
68              print("Exiting at iteration ", tt, "/", MAX_ITERATIONS, "
                    Condition on epsilon reached")
69              sys.stdout.flush()
70
71          break
72
73      if tt in range(0, MAX_ITERATIONS, 100):
74          if rank == 0:
75              print("Iteration ", tt, "/", MAX_ITERATIONS)
76              sys.stdout.flush()
77      ITERATION_DONE = tt
```

When consensus is reached, the theta values are printed to user, then all data are sent to rank 0 for centralized calculations and plot result.

Chapter 2

Results of simulations

To verify the correctness of the software, a couple of simulations were run, divided into two parts:

- Minimization of the Softmax function to prove the convergence to the optimal value
- Application of the minimization algorithm to find the optimal coefficients and prediction on the test dataset

2.1 Minimization of the Softmax function

The simulation has been carried out using a random directed graph made up of 17 agents, as shown in figure 2.1.

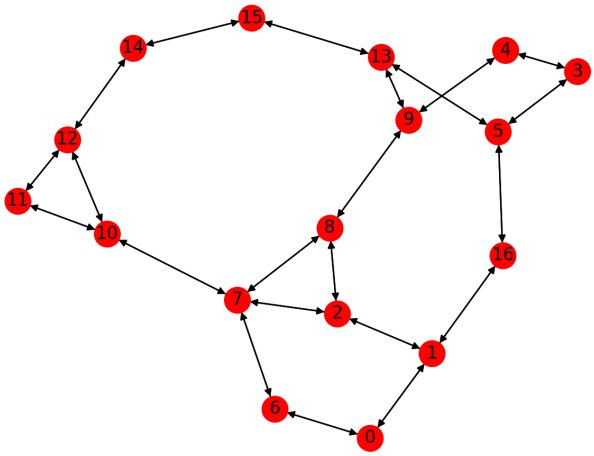


Figure 2.1: Communication graph used for the simulation.

For completing this simulation, a diminishing step-size has been used, with the following formulation:

$$\alpha^k = 0.01 \left(\frac{1}{k}\right)^{0.4} \tag{2.1}$$

with k indicating the current iteration.
The problem to be solved is the one formulated in 1.7. Let's suppose to indicate the whole dataset as S. Each agent i can access to a limited set s_i of examples contained in S. To each agent is given a set s_i, chosen as:

$$S = \bigcup_{i=1}^{17} s_i \tag{2.2}$$

In the simulation, the training set S is composed by 120 examples, split into set s_i of 6 or 7 examples, chosen in order to equation 2.2 hold.
The iterations run are 15000, sufficient enough to see the function approaching the convergence, but not sufficient enough to reach the minimum value of the function, calculated with MATLAB to be 8.945. The figure 2.2 shows in a logarithmic scale how the algorithm tends to minimize the cost value at each iteration.

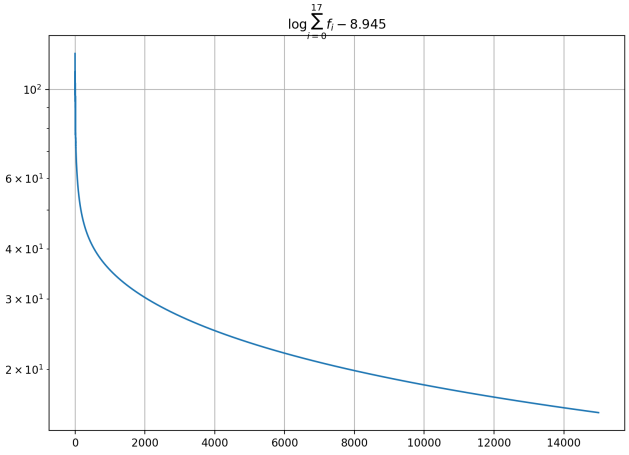


Figure 2.2: Value of the normalized cost function in a logarithmic scale over all the iterations.

The value of the cost function is shown in figure 2.3 in a linear scale too, so it can be seen how the algorithm approaches the minimum value Θ^* in order to have the minimum of the problem 1.7.

As can be seen in figure 2.4, all the agents try to reach the consensus for each component of the local minimum of the problem.

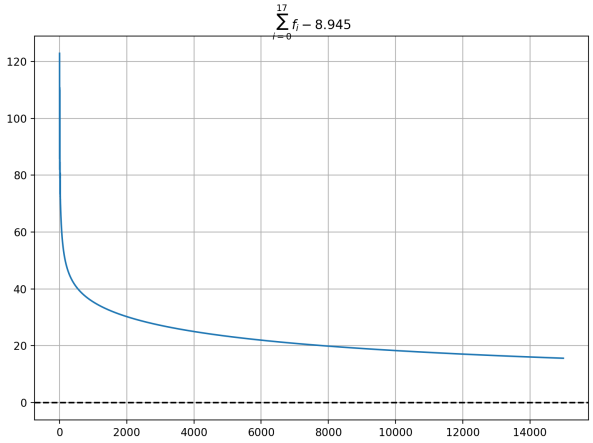
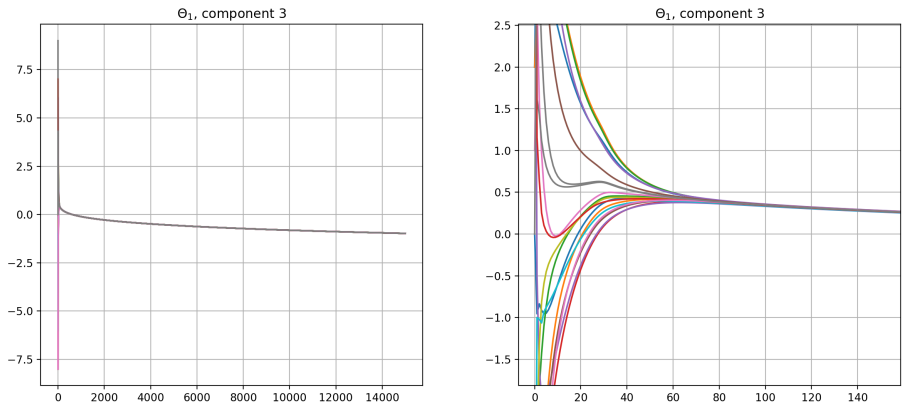


Figure 2.3: Value of the normalized cost function in a linear scale.

To better see the consensus, in this simulation the initial condition have been chosen to be random integer number between -10 and $+10$. With this choice is more visible the trend if the agents that try to reach consensus.



(a) Overall trend over all the iterations (b) Detail for the first 140 iterations

Figure 2.4: Consensus on the third component of Θ_1

2.2 Dataset, graph description and minimization function

This dataset is composed of 150 instances, 120 used for training, the rest for tests. The instances contain 3 classes, each representing a type of Iris flower. Every instance has 4 features, sepal length, sepal width, petal length, petal width expressed in *cm*. We tried different types of graphs. These graphs are all strongly connected and the weight matrices for the nodes are doubly stochastic, as per the assumptions of convergence of the algorithm described in Chapter 1. The results discussed in this chapter, if not differently noted, refer to cyclic graphs with a variable number of nodes. The program can minimize all kinds of loss functions. As shown in Chapter 1.2, the quadratic and exponential functions can also be used. These last 2 functions don't guarantee useful results and/or convergence. The minimization function used in this chapter is the one described in Chapter 1.1.2, softmax.

2.3 Performance

There are some key factors that influence *the computational time*, *the numbers of iterations necessary* and *the accuracy of the results*.

2.3.1 Number of nodes

The Python program, thanks to the MPI platform, is capable of running on an arbitrary number of nodes. It was tested on as little as 2 nodes to as many as 60 nodes, which means that every node was processing the data of 2 instances (120 instances divided into 60 nodes). The best performances are obtained when the number of nodes corresponds to the number of physical cores of the machine where it runs. When the number of nodes exceeds greatly the number of physical cores, the resources are oversubscribed. In this case, the performances degrade notably as the nodes compete for cache and memory and the processors' schedulers are put in a difficult situation. On a 4-core test machine, a computation with 5000 iterations and 30 nodes is done in 5 minutes. The same machine can do the same number of iterations, but with 60 nodes, in 15 minutes. Therefore, to show the scalability of the software, the following tests will be shown on a 4 nodes set-up and a 17 nodes setup (the same of figure 2.1) .

2.3.2 Epsilon

This is a small constant used as stop condition. If the result of the current calculation differs less than epsilon from the previous, the algorithm is

stopped.

2.3.3 Learning rate

The step-size alpha plays a big role in the speed of convergence of the algorithm. There are 3 kinds of step-size. Fixed, diminishing and adaptive (Armijo). For reasons not discussed in this paper, it's not possible to use Armijo rule in a distributed problem.

2.3.4 Initial condition

The agents should start with an initial condition, expressed in the code with x0. This initial condition is the state from which the agents start to compute. The program was tested with random initial conditions for all agents and the consensus was still reached. The garantee the repeatability of the experiments, the initial condition in the tests is always set to 1.

2.4 Four Nodes Setup

2.4.1 Fixed step-size

We will first deal with a simpler fixed step-size. With an epsilon equal to 0.001 (10^{-3}):

Value of fixed step-size	**Iteration required**	**Execution time in s**	**Wrong guesses o.30**
0.5	overflow	alpha too big	-
0.1	>10000	>15	2
0.05	>10000	>15	1
0.01	1968	2.8	1
0.005	1558	2.3	1
0.001	2114	3.1	0
0.0005	1619	2.3	2
0.0001	527	0.7	14

These results show a general truth about the step-size. If it is too little, the learning process proceeds in a very slow way and it requires a huge amount of iterations. If the learning rate is too high, the gradient descent will most probably overshoot the minimum and it will not converge. Through trial and error, the step-size 0.001 was identified, it allows reaching good performance and accuracy. In fact, in only 3.1 seconds, we can make predictions with no errors, using our 30 instances test dataset.

2.4.2 Diminishing step-size

The diminishing step-size implemented in the code is in this form: TODO: SISTEMARE FORMULA

$$\alpha = const \left(\frac{1}{tt}\right) exp \tag{2.3}$$

Again, several tests were run by tweaking the multiplying constant and the exponent.

psi_coeff	**alpha_exp coefficient**	**Iteration required**	**Execution time in s**	**Wrong guesses o. 30**
1	0.01	overflow	-	-
1	0.1	overflow	-	-
0.1	0.01	>10000	>15	1
0.1	0.5	349	0.5	0
0.1	0.1	>10000	>16	1
0.01	0.01	1852	2.7	1
0.01	0.1	1259	1.8	1

The best result is obtained in only 349 iterations, with 0.1 and 0.5 as multiplicative constant and exponent respectively. This is done in roughly half of a second, obtaining no error. The accuracy is worst then the previous result, but this is obtained in a fraction of the time needed to obtain 0 error with a fixed step-size. A difference of 2 or 3 seconds may not seem important using the Iris Dataset, with a small amount of calculations. In a set-up where a bigger number of calculations and bigger dataset are involved, one may appreciate the advantages of this faster approach.

2.5 Seventeen Nodes Setup

These are the results for the setup shown in figure 2.1.
The computation times are greatly larger, the tests were executed on a quad-core machine, MPI oversubscribed the resources and the CPU scheduler was put at hard work.
The results are still very interesting.
The optimal step-size is different from the ideal step-size of the 4 nodes setup. Only through several tests and experience is possible to find a good step-size.

psi_coeff	**alpha_exp coefficient**	**Iteration required**	**Execution time in s**	**Wrong guesses o. 30**
0.1	0.1	>10000	>440	2
0.5	0.1	>1000	>440	2
0.9	0.1	>10000	>440	2
0.01	0.1	1894	83	2
0.1	0.5	698	30	2
0.5	0.5	1017	44	1
0.9	0.5	2409	107	0
0.01	0.5	318	13	14
0.1	0.01	>10000	>440	1
0.5	0.01	>10000	>440	2
0.9	0.01	>10000	>440	2
0.01	0.01	3717	164	2

TODO: AGGIUNGERE GRAFICI

Conclusions

In this work it has been resolved a Multinomial Logistic Regression problem using MPI in Python. Each agent used a Distributed Sub-gradient method to update its own estimate of optimal solution.

Bibliography

[1] A. Nedic and A. Ozdaglar. Distributed subgradient methods for multi-agent optimization. *IEEE Transactions on Automatic Control*, 2009.

[2] Stanford. Softmax regression. Available at `http://ufldl.stanford.edu/tutorial/supervised/SoftmaxRegression/`.

[3] Wikipedia. Multinomial logistic regression. Available at `https://en.wikipedia.org/wiki/Multinomial_logistic_regression`.