

Open MPI implementation of K-Nearest Neighbors classifier

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Abstract— The goal of this project is to provide an efficient implementation of the K-Nearest Neighbors (Machine Learning) algorithm, that exploits multiple CPUs architectures, using Open MPI (on C++). Starting from a serial implementation, the code has been modified to work in parallel, obtaining an improvement in terms of performances, and so, a significant speedup (compared with the standard serial version). An a priori study of available parallelism has been conducted, to identify the parts of the serial code that could have been parallelized. To better understand how this implementation scales, two dimensions have been varied: the datasets sizes, and processors number. So doing, the code has been executed on Google Cloud Platform virtual instances, to exploit the whole computational power of a cluster of machines cooperating one with each other.

Keywords— K-Nearest Neighbors • Machine Learning • Parallelization • Open MPI • Performances • Google Cloud Platform

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1. WHAT IS K-NEAREST NEIGHBORS

Nowadays Machine Learning (ML), a branch of Artificial Intelligence (AI) that automates the construction of analytical models based on the idea that systems can learn from data without the need for human intervention, is becoming used in many different application fields, especially

to build efficient models which help humans in taking decisions, understanding interesting patterns, and so on.

The problems that Machine Learning can efficiently solve belong in two different macro-groups: supervised learning (classification, regression) and unsupervised learning (clustering, dimensionality reduction). The former group uses labeled datasets to train algorithms to find which are the most impactful features for a given phenomenon outcome (categorical or continuous values). The latter, instead, uses unlabeled datasets to analyze and discover hidden patterns or data groupings.

The K-Nearest Neighbors algorithm (KNN) is falling into the supervised learning methods, and is based on proximity to make classifications or predictions of an individual data point. It works particularly well when the assumption that similar points can be found near one another is true.

The report threaten version can solve classification problems, but it can be easily extended (properly modifying it) to solve also regression problems.

Its basic working principle is to assign the class label to a given point on the basis of a majority vote, considering its K nearest neighbors. Those K points are obtained by performing a selected distance function (e.g: Euclidean, Manhattan, Minkowski or Hamming).

Obviously, each distance function provides different results. In this implementation, the Euclidean distance is the standard (and only) one.

In order to display its behavior, a simple example, where both the classes and features number are just two, has been chosen [1]. A question that might come to your mind is:

- What is the class of the unclassified point?

Based on what stated previously, if the number of considered neighbors (K) is equal to three the most occurrent class is the green one, otherwise considering six it would have been red. The described working flow is the same considering a more

complex example.

Even the choice of the value of the parameter K is a critical aspect, since it can lead to over-fitting (low K) or under-fitting (high K). It should be properly tuned, since it will largely depend on the input data, as data with more outliers or noise will likely perform better with higher values of K. Clearly it should have some sense considering very far (high K, course of dimensionality) points.

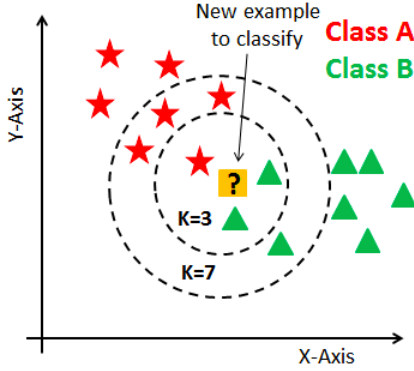


Fig. 1: Simple K-Nearest Neighbors problem [10]

2. SAMPLE DATASETS GENERATION

Even though the implementations that will be discussed in details in the following sections are capable of perform classification even on real case datasets (as will be shown on the well-known Iris dataset [9]), the objectives of this analysis are more biased on execution performances with respect to Machine Learning in a strict sense (the goal is not to find the best configuration for a KNN classifier in a specific field of study).

So, even a general purpose dataset (with not a real meaning of the features representing a specific characteristic for that sample of a given class) can be considered as good as benchmark to test how the code behaves in terms of performances by considering different aspects such as: the number of samples (dataset dimension), the number of classes, the number of features for each class (still related to the dataset dimension), and whether to apply Min-Max scaling.

In order to cover this aspect, a specific Python script has been implemented [7].

3. SERIAL IMPLEMENTATION

In the section, it will be discussed how the serial version of the KNN algorithm has been implemented from scratch, using C++ [6].

Parameter	Description
trainFile	Path of train file
nTrainSamples	Number of train points to use
testFile	Path of test file
nTestSamples	Number of test points to use
K	Number of neighbors
nFeatures	Number of features for each sample
nClasses	Number of classes

Table 1: Parameters of the serial version

The code can be described as a set of consequent steps, in order to perform classification on a general dataset. The final objective is, given some parameters [1] (a more detailed description can be found in the project's README file [4]), to obtain train and test accuracy of a KNN model.

More precise classification performance metrics should have been used (e.g., to understand whether the selected model is more biased on recognizing a class with respect to another), but this is not the actual purpose of the project.

In order to obtain the test accuracy (the same line of reasoning follows for train accuracy), the following steps are performed one after the other:

- Consider each test sample and compute the Euclidean distance (1) with respect to all the train samples
- Consider the most occurrent class of K-Nearest Neighbors points of each test sample and assign it to the predicted test sample class
- Compare the actual class of the test sample with the predicted one, if the values are equal the sample has been correctly classified (classification accuracy consequently increases), otherwise not
- Divide the number of correctly classified test points by the total number of test points, multiply for 100, which represents the test accuracy

N-dimensional Euclidean distance formula The used distance formula is the one depicted below.

$$d(p, q) = \sqrt{\sum_{i=1}^n (q_i - p_i)^2} \quad (1)$$

Where p and q are respectively a train and test sample, whereas n is the number of features that the two considered samples have.

The discussed serial algorithm has been applied also on the already cited Iris dataset (considering a train-test split of 80%-20% and fine-tuning the K parameter - using a random search approach), in order to show that it can work properly also with datasets used daily by the data scientist community. For this simple classification problem, both train and test accuracies are almost 97% (neither over-fitting nor under-fitting, since the discrepancy between the two is negligible).

Example on how the script can be executed, once compiled, on the Iris dataset, considering ten neighbors:

```
./knn-serial.o ../Datasets/train.txt
120 ../Datasets/test.txt 30 10 4 3
```



Fig. 2: Visual representation of the different iris classes. It is well-known that the two more distinguishable features between all those iris types are sepal and petal [8]



Cost associated with each task of the serial code, in terms of number of instructions For what concerns the serial implementation, an a priori estimate on the number of instructions needed to conclude specific tasks has been conducted, in order to better understand which are the functions that needed more parallelization (if possible), since more computationally expensive.

The results of that analysis are shown in the following table, which has been obtained by looking directly at the code of the serial version (they can also be checked more accurately by using a specific profiler tool such as Valgrind or Gprof).

Task	Cost (# of instructions)
Euclidean distance	$N_{Features} + 2$
Sorting	$n_{TrainSamples} * \log(n_{TrainSamples})$
KNN prediction	$n_{TrainSamples} * EuclDist + Sort + 3 * n_{Classes} + K$
Array calculus	$n_{TestSamples} * KNN_{Prediction} + 2$
Read train samples	$1 + n_{TrainSamples} * (2 + n_{Features})$
Read test samples	$1 + n_{TestSamples} * (2 + n_{Features})$
Initialization	20

Table 2: Estimate of the number of instruction executed, for each function of the serial implemented version

An aspect that can be pointed out is that typically, in the Machine Learning field, the number of samples belonging into the train set are substantially more with respect to the one appertaining to the test set.

This choice comes from a very linear reasoning: because the test set's job is only evaluating the trained model's performance on unseen data (while the model learning happens on train data). Learning the model is a far more complex task than evaluating the model performance. If the training set is small, the model tends to overfit and may not generalize well to new data patterns that are not seen in training data. So model performance typically improves as training dataset size increases (until a certain point, when the gains get saturated).

So, the cost as the number of instructions associated with each task that regards the test set is lower if compared with the cost of the same tasks working with the train set.

4. AVAILABLE PARALLELISM

In this section, it will be briefly discussed the expected improvement in terms of performances of parallelizing the serial solution described previously.

The serial version code has been analyzed discarding the less relevant (neither critical nor crucial) parts, such as: the checks on the parameters that can be passed to the `main()` function; the import of the libraries, and the both global variables and the sample (`struct`) definition. The only fraction of code that cannot be efficiently, nor simply, be parallelized is the reading of the two datasets (train and test). All the other functions can exploit multiple CPUs architectures (how they have been parallelized is explained in the next section).

Amdahl's law In order to understand the plausible speedup which can be obtained parallelizing the serial version, the Amdahl's law has been used. Its formula is the following one:

$$Speedup(N) = \frac{1}{S + \frac{P}{N}} \quad (2)$$

Where N is the number of CPUs used, S is the fraction of the code that cannot be parallelized (serial execution), while P the fraction that can be parallelized (recall that $P + S = 1$).

By looking at the previous table it can be noticed that the number of iterations for each task, among other things, is strongly correlated with the dataset dimension (the number of samples to be considered both in train and test).

Since the speedup depends on the portion of serializable (and non) fraction of code and those two depend on the number of samples, it can be noticed that the speedup does not change only with the number of cores (which can equally spread the work), but also on the number of samples (neglecting the number of features for each sample, the K and the number of classes).

The serializable code fraction diminishes with the increasing of the dimension of the dataset (tends to zero, as shown on the next graph), so consequently the speedup should increase linearly with the cores number.

Actually, differently from what discussed from the "theoretical" point of view, what is expected is that the dimension of the dataset impacts negatively (to be valued how much) the execution time, since the data transmission between master and slaves depends (grows proportionally) on the amount of train and test of samples.

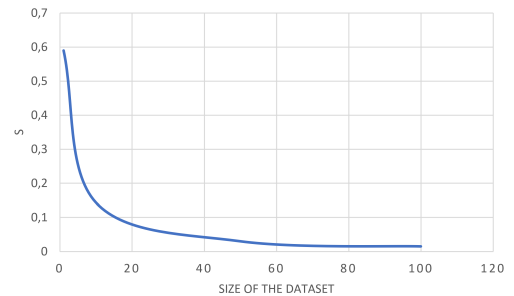


Fig. 3: Theoretical fraction of code that cannot be parallelized, in relation to the size of the dataset

5. OPEN-MPI IMPLEMENTATION

Parallelize or distribute a task, such that the same operation can be executed on different nodes, is considered a must in lot of field, let's just think for example about the Big Data analysis (have a look at Apache Spark if interested in that topic). How can be possible that a single CPU can, in a computationally feasible time, complete a task? Exploiting the parallelism of a single machine can drastically reduce the execution time of that task, if the parallelization procedure has been well-designed, but it suffers from the issue of the lack of possible memory allocation.

For that specific purpose, using distributed systems allowed to exploit not only vertical scalability (so to use all the computational power provided by a single machine, that, as imaginable, is limited), but also the possibility to use the whole computational power of multiple machines coping together to achieve a specific goal.

In order to do that, there are basically two major ways: shared memory systems or distributed memory system. The two mentioned options have both advantages and disadvantages.

tages.

Designing those solutions is not as easy as it seems to be, for multiple factors such as load balancing and data partitioning. In this specific case, using Open MPI (Message Passing Interface) allows implementing, test and run a solution on a distributed memory system. Through messages sending between a master node and its slaves, it is possible to handle the spread of data between multiple machines, where each one of them has its own memory and its own computational power to use.

The code that will be discussed in this section, has been implemented by considering the serial version and distributing it using Open MPI, still with C++ [5].

Even in this particular case, the implementation can be described as a set of consequent steps, in order to perform classification on a general dataset. It takes as input the already discussed parameters shown in the serial implementation, and it prints as output the train and test accuracy of the selected KNN model, on the specified datasets. Furthermore, to facilitate the performance analysis, the execution times and configurations of parameters have been stored in specific files.

Two very important additional parameters are the number of CPUs on which run the code, but MPI also gives the possibility to specify a host-file, that will be useful to perform tests on different clusters of machines.

To obtain the test accuracy (almost the same line of reasoning follows for train accuracy, except some very little differences), the following steps are performed:

- The master node reads both the train and test datasets, then scatters to all the slaves a portion of the test dataset, and broadcasts all train samples (already done since used also to assess the train accuracy)
- Each slave works on a fraction of the test dataset to assess its own accuracy. This accuracy assessment of each node is basically the same one as already summarized in the serial implementation
- In case the fraction of data is not divisible by the number of slaves, the master node works also on the remaining fraction of samples. Furthermore, the accuracy calculated by each slave weights differently (since just one machine has computed also the accuracy on the reminder)
- Finally a reduce function is performed by the master to obtain the overall test accuracy, gathering all the slaves accuracies (3)

This version is obviously consistent with the serial one (maintaining fixed the dataset and all the other parameters), but also by increasing the number of CPUs on which this code is executed. Example on how the script can be executed, once compiled, on a relatively big dataset (120K samples, 100 features per sample), considering still ten neighbors and a cluster that has at least 16 virtual CPUs available:

```
mpirun --use-hwthread-cpus
--hostfile hostfile -n 16
knn-distributed.o
../Datasets/train.txt 100000
../Datasets/test.txt 20000
10 100 6
```

Overall accuracy (distributed case) The used overall accuracy is the one depicted below.

$$Acc_{tot} = \frac{1}{N} \left(\sum_{k=1}^C Acc_k * \frac{N}{C} + (Acc_{rem} * N \bmod C) \right) \quad (3)$$

Where N is the total number of samples, C is the total number of CPUs available, Acc_k is the accuracy obtained by the k -th CPU, whereas Acc_{rem} is the accuracy obtained by a node on the reminder (whether $N \bmod C \neq 0$).

6. PERFORMANCE ANALYSIS

Once treated in detail the discussion of the distributed implementation with Open MPI, it is necessary to consider how well this implementation is in terms of performance, more specifically for what concerns the execution time.

The testing and debugging tasks has previously done on local machines. Once different tests passed without bug occurrence, the code has been moved to the latter described Google Cloud Platform (GCP) clusters. GCP is a suite of cloud computing services offered by Google that provides a range of infrastructure and platform services, including computing, storage, networking, big data, machine learning, and security, making it a popular choice for businesses of all sizes.

For the KNN distributed calculations and performance tests through the GCP, four different clusters have been created:

- **Fat cluster:** three e2-highcpu-8 (8vCPU, 8GBRAM)

Intra-regional: same region (Central America)

Infra-regional: different regions (1 Central Europe, 1 East Asia, 1 West America)

- **Light cluster:** six e2-small (2vCPU, 2GBRAM)

Intra-regional: same region (Central America)

Infra-regional: different regions (2 Central Europe, 2 East Asia and 2 West America)

In order to automate the tests, a bash script [2] has been created. It considers an already generated dataset, with the following requirements: at least 25K overall samples, 50 features and 4 classes (the dataset can be further increased, but since the tests started by examine the classifier using just one CPUs it would have taken too much time to perform this task using just one calculation unit on a huge dataset).

The user can select whether to run the tests (no matters if intra or infra regional) on the light or fat cluster and then all the tests are being performed by varying the number of samples considered and the number of cores on which the code is executed. The other parameters (e.g. the number of features, K , ...) have clearly an influence on the overall execution time, but in order to keep simple and easily understandable the performance analysis discussion it has been chosen to vary only the two already mentioned parameters (number of cores and number of samples).

Each time a single test is executed, a new row is added into a .csv file, that contains all the execution details (number of samples, number of cores, execution time) for one specific cluster, and then for simplicity the different execution details

have been moved to single files, for the already discussed clusters, in a specific folder [3].

The execution detail files have been used to conduce the performance analysis and to generate all the graphs that will be later shown (through a Jupyter Notebook file [1]).

Now, it will be performed a description on strong and weak scalability, considering the execution times gathered for each specific cluster.

What does the term weak and strong scalability means? Strong scalability refers to the ability of a parallel algorithm to maintain a fixed problem size and reduce the computation time as more processors are added. In other words, if the number of processors is doubled, the computation time should be halved, while keeping the size of the problem fixed. This means that the efficiency of the algorithm is maintained even as more processors are added. Strong scalability is important when dealing with a fixed amount of data that needs to be processed as quickly as possible.

On the other hand, weak scalability refers to the ability of a parallel algorithm to maintain a fixed computation time as more processors are added, while increasing the problem size. In other words, if the number of processors is doubled and also the size of the problem, the computation time should remain the same. This means that the algorithm is able to handle larger problems while maintaining a constant level of efficiency. Weak scalability is important when dealing with large and complex problems that require more resources as the problem size increases.

a. Fat cluster

A fat cluster, consisting of few machines with significant computational power, can be beneficial for various reasons, including:

- **High Performance:** designed for high-performance computing (HPC), and the powerful machines that make up the cluster can handle complex and resource-intensive workloads. With more powerful machines, a fat cluster can provide high-speed data processing, faster rendering times, and other demanding computing tasks
- **Reduced Network Latency:** there are fewer machines and network connections to manage, resulting in reduced network latency. This can be particularly important for tasks that require a lot of data transfer or low-latency communication between nodes
- **Easier Management:** easier to manage than many smaller machines. With fewer machines, system administrators can spend less time on maintenance tasks and more time optimizing the system for performance
- **Improved Security:** can be more secure than a light cluster because there are fewer machines to secure and monitor. With fewer machines, system administrators can focus on implementing robust security measures, such as firewalls and intrusion detection systems, to protect the cluster from cyber threats
- **Cost-effective:** can be more cost-effective than a light cluster in some scenarios. For example, if the workload requires a lot of memory or other resources, it may be more cost-effective to use a few powerful machines with high-end hardware, rather than many smaller machines

Overall, a fat cluster consisting of a few powerful machines can provide high performance, reduced network latency, easier management, improved security, and cost-effectiveness in certain scenarios. It is well-suited for HPC workloads that require a lot of processing power and resources, and can provide a more streamlined and manageable infrastructure compared to a light cluster.

1. Intra-regional

As already described, one of the four created clusters was a fat cluster, with few powerful machines that are placed within the same geographical area.

Strong scalability has been studied through the computation of speedup (4). The speedup of the distributed algorithm can be considered as good, since as the number of cores increases (no matter the amount of data to process), the speedup increases as well (not linearly, but close to it). The fact that the speedup is not linear can be due to data synchronization and so the data transfer phase improves negatively on the overall performances (as expected, and already pointed out previously). Another aspect, not to be neglected, is that maintaining the number of samples small and increasing the number of cores does not work as good as the other cases. Since the single node has fewer work to do, the time spent to send the data to all nodes has an higher impact on the total time of execution, and so, on the speedup.

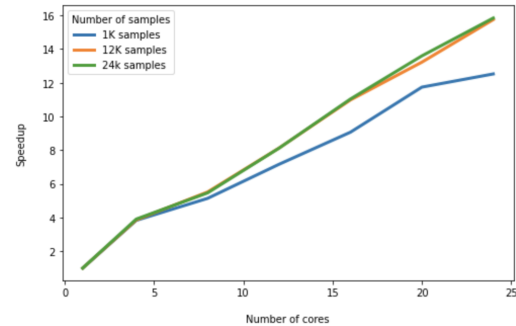


Fig. 4: Strong scalability for the fat intra-regional cluster

Speedup, alternative formula Another well-known formula for the calculation of the speedup is the following one:

$$Speedup(N) = \frac{t(1)}{t(N)} \quad (4)$$

Where $t(1)$ is the amount of time needed to complete the task with one process, whereas $t(n)$ is the amount of time to complete the same task with N processing units.

Whereas, for the weak scalability, the performances have been measured in terms of efficiency (5).

Increasing the load per core, drastically decreases the overall performances. Especially if the number of virtual CPUs is becoming greater than the one that a single machine contains. This can be due to the fact that the transfer of data within the same machine and different machines costs differently (a lot more in the second case). Furthermore, if the dimension of the dataset is reduced, also the efficiency decreases (fewer samples, a lot of machines so more data exchange than effective useful calculation).

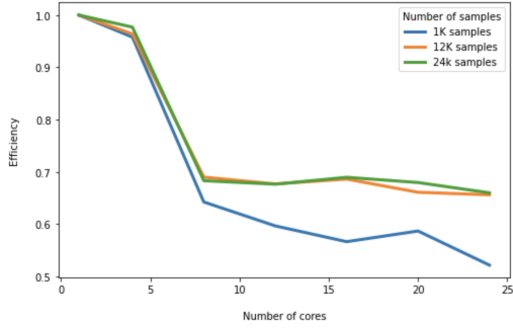


Fig. 5: Weak scalability for the fat intra-regional cluster

Efficiency A used formula for the calculation of the performances for weak scalability is the following:

$$Efficiency(N) \approx \frac{Speedup}{N} \quad (5)$$

Where N is the number of virtual CPUs used [11].

2. Infra-regional

In this section, it will be discussed whether there is a significant difference between the infra-regional and intra-regional fat cluster performed tests. In order to do so, it has been firstly calculated the difference between the execution times of the fat infra-regional cluster and intra-regional cluster (considering the same test configuration), then divide this difference by the average of the two execution time values (for infra and intra regional).

This operation showed that there is not a huge difference between the two cases (Mean: 0.015 , Variance: 0.00037), so using an infra-regional or intra-regional fat cluster does not make any particular difference.

This behavior can be strange at first glance, but the geographical distance between two nodes is not the only factors that affects the time to transfer (latency), because this depends also on many other factors like the channel capacity, the network congestion, the number of hops, and so on. A possible hypothesis is that Google has deployed an infrastructure that has a really high transfer rate and so the geographical distance does not affect so much the execution time.

b. Light cluster

A light cluster, consisting of a lot of machines with lower computational power, can also offer several benefits for certain use cases, including:

- **Cost-effective:** more cost-effective than using heavy ones, as they tend to consume less power and require fewer hardware resources. This can result in lower operating costs and can also help reduce upfront capital expenditures
- **Scalability:** highly scalable, as it is easy to add or remove machines as needed. This can help organizations quickly adapt to changing workload demands without over-provisioning resources CPUs
- **Resilience:** can be more resilient than a smaller number of heavy machines. If one machine fails, the remaining machines can pick up the workload, minimizing downtime

- **Flexibility:** it is possible to run different types of workloads on different machines, depending on the specific requirements of each workload. This can result in better resource utilization and can help reduce costs
- **Energy-efficient:** Lightweight machines tend to be more energy-efficient than heavy ones, as they consume less power. This can help organizations reduce their carbon footprint and energy costs

Overall, a light cluster consisting of many lightweight machines can provide cost-effective scalability, resilience, flexibility, and energy efficiency. It can also help organizations quickly adapt to changing workload demands and reduce their overall operating costs.

1. Intra-regional

Another cluster was the one in which lot light-weighted machines are placed within the same geographical area.

Strong scalability has been studied through the computation of speedup (4).

The speedup of the distributed algorithm can be considered as good (similarly to the fat cluster), since as the number of cores increases (no matter the amount of data to process), the speedup increases (still in this case not linearly). Please notice that in this case the maximum number of cores exploited was twelve (not twenty-four as the fat one), so the two behavior can be considered very similar (so also the conclusions are the same).

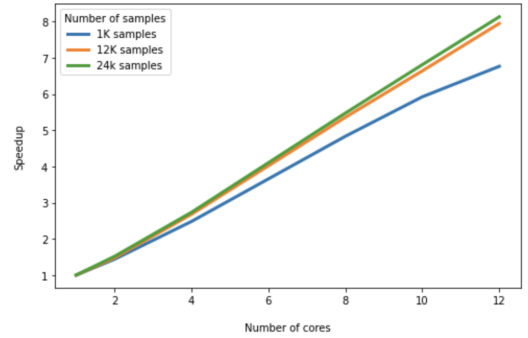


Fig. 6: Strong scalability for the light intra-regional cluster

Whereas, for the weak scalability, the performances have been measured in terms of efficiency (5).

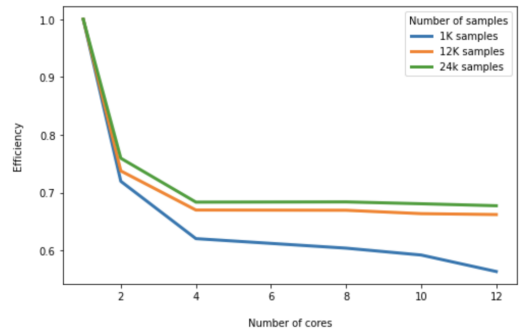


Fig. 7: Weak scalability for the light intra-regional cluster

The overall obtained results for the weak scalability are similar to the one of the fat intra-regional cluster, except



for the fact that the efficiency starts degrading before (hypothesis that the transfer of data within the same machine and different machines costs differently, more in the second case). Even in this case, if the dimension of the dataset is reduced, also the efficiency decreases (fewer samples, a lot of machines so more data exchange than effective useful calculation).

2. Infra-regional

Still, for light cluster, it will be discussed whether there is a significant difference between the infra-regional and intra-regional fat cluster performed tests. In order to test it, the same calculus as described previously has been considered.

The operation showed that there is not a huge difference between the two cases (Mean: 0.012 , Variance: 0.00347), so using an infra-regional or intra-regional light cluster does not make any particular difference (note that the variance is higher with respect to the case of fat cluster).

7. CONCLUSIONS

The proposed distributed implementation, allowed achieving a decent speedup for both strong and weak scalability (even if lower than linear, which is considered the "Holy Grail"), both for fat or light cluster infra-regional and intra-regional cluster.

In the test that have been performed it seems that opting for a fat cluster (infra-regional or intra-regional), does affect more positively the execution time (especially if possible working within the same machine, otherwise time transfer cost can be noticed).

In conclusion, the proper configuration depends on multiple factors. If fewer data to process, is better, opting for a light cluster (not so powerful neither with a huge RAM), whereas if there are far more data to process is better using a fat cluster (the power needed also in this case depends on the specific classification task), also in order to limit the amount of data transmitted.

8. CONTRIBUTIONS

In the following table, it is described to which task each project's member have contributed.

Author	Major contribution
F. Amato	Report + GitHub repo's description
	Datasets generation
	Serial + parallel implementations
	Code testing (also GCP) + debugging
D. Ligari	Performance + scalability analysis
	Available parallelism + Ahmdal's law
	Code testing + debugging
	GCP clusters configuration + testing
	Performance + scalability analysis

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