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Alla mia famiglia…

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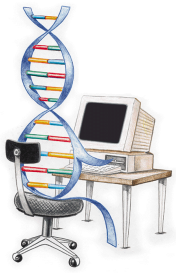
1 Introduction



Computing has rapidly established itself as essential and important to many branches of science, to the point where *computational science* is a commonly used term. Indeed, the application and importance of computing is set to grow dramatically across almost all the sciences. Computing has started to change how science is done, enabling new scientific advances through enabling new kinds of experiments. These experiments are also generating new kinds of data of increasingly exponential complexity and volume. Achieving the goal of being able to use, exploit and share these data most effectively is a huge challenge.

It is necessary to merge the capabilities of a file system to store and transmit bulk data from experiments, with logical organization of files into indexed data collections, allowing efficient query and analytical operations. It is also necessary to incorporate extensive metadata describing each experiment and the produced data.

Rather than flat files traditionally used in scientific data processing, the full power of relational databases is needed to allow effective interactions with the data, and an interface which can be exploited by the extensive scientific toolkits available, for purposes such as visualization and plotting.

Different disciplines require support for much more diverse types of tasks than we find in the large, very coherent and stable virtual organizations. Astronomy, for example, has far more emphasis on the collation of federated data sets held at disparate sites (Brescia et al. 2010). There is less massive computation, and large-scale modeling is generally done on departmental High Performance Computing (HPC) facilities, where some communities are formed of very small teams and relatively undeveloped computational infrastructure. In other cases, such as the life sciences, the problems are far more related to heterogeneous, dispersed data rather than computation. The harder problem for the future is heterogeneity, of platforms, data and applications, rather than simply the scale of the deployed resources. The goal should be to allow scientists to explore the data easily, with sufficient processing power for any desired algorithm to process it. Current platforms require the scientists to overcome computing barriers between them and the data (Fabbiano et al. 2010).

Our convincement is that most aspects of computing will see exponential growth in bandwidth, but sub-linear or no improvements at all in latency. Moore's Law will continue to deliver exponential increases in memory size but the speed with which data can be transferred between memory and CPUs will remain more or less constant and marginal improvements can only be made through advances in caching

technology. Certainly Moore's law will allow the creation of parallel computing capabilities on single chips by packing multiple CPU cores onto it, but the clock speed that determines the speed of computation is constrained to remain limited by a *thermal wall* (Sutter 2005). We will continue to see exponential growth in disk capacity, but the factors which determine latency of data transfer will grow sub-linearly at best, or more likely remain constant. Thus computing machines will not get much faster. But they will have the parallel computing power and storage capacity that we used to only get from specialist hardware. As a result, smaller numbers of supercomputers will be built but at even higher cost. From an application development point of view, this will require a fundamental paradigm shift from the currently sequential or parallel programming approach in scientific applications to a mix of parallel and distributed programming that builds programs that exploit low latency in multi core CPUs. But they are explicitly designed to cope with high latency whenever the task at hand requires more computational resources than can be provided by a single machine. Computing machines can be networked into clouds or grids of clusters and perform tasks that were traditionally restricted to supercomputers at a fraction of the cost. A consequence of building grids over wide-area networks and across organizational boundaries is that the currently prevailing synchronous approach to distributed programming will have to be replaced with a fundamentally more reliable asynchronous programming approach. A first step in that direction is S*ervice-Oriented Architectures* (SOA) that has emerged and support reuse of both functionality and data in cross-organizational distributed computing

settings. The paradigm of SOA and the web-service infrastructures facilitate this roadmap (Shadbolt et al. 2006).

Traditionally, scientists have been good at sharing and reusing each other's application and infrastructure code. In order to take advantage of distributed computing resources in a grid, scientists will increasingly also have to reuse code, interface definitions, data schemas and the distributed computing middleware required to interact in a cluster or grid. The fundamental primitive that SOA infrastructures provide is the ability to locate and invoke a service across machine and organizational boundaries, both in a synchronous and an asynchronous manner. The implementation of a service can be achieved by wrapping legacy scientific application code and resource schedulers, which allows for a viable migration path (Taylor et al. 2007). Computational scientists will be able to flexibly orchestrate these services into computational workflows. The standards available for service design and their implementation support the rapid definition and execution of scientific workflows. With the advent of abstract machines, it is now possible to mix compilation and interpretation as well as integrate code written in different languages seamlessly into an application or service. These platforms provide a solid basis for experimenting with and implementing domain-specific programming languages and we expect specialist languages for computational science to emerge that offer asynchronous and parallel programming models while retaining the ability to interface with legacy FORTRAN, C, C++ and Java code.

The original work of the present thesis consists of the design and development of a multi-purpose genetic algorithm implemented with the GPGPU/CUDA parallel

computing technology. The model comes out from the machine learning supervised paradigm, dealing with both regression and classification scientific problems applied on massive data sets. The model was derived from the original serial implementation, named GAME (Genetic Algorithm Model Experiment) deployed on the DAME[1] Program hybrid distributed infrastructure and made available through the DAMEWARE[2] data mining web application. In such environment the GAME model has been scientifically tested and validated on astrophysics massive data sets problems with successful results (Brescia et al. 2011b). As known, genetic algorithms are derived from Darwin's evolution law and are intrinsically parallel in its learning evolution rule and processing data patterns. The parallel computing paradigm can indeed provide an optimal exploit of the internal training features of the model, permitting a strong optimization in terms of processing performances. Such requirement is particularly important in case of real problem cases having to deal with massive data sets, such as, for instance, the data quality mining of observed and telemetry data coming out from astronomical ground- and space-based instrumentation. We intend to perform experiments of GPU-based GAME model on EUCLID[3] Mission, a multi-wavelength space telescope, provided by European Space Agency (ESA), foreseen to be launched in 2019, in which our DAME group is leading the data quality science team.

[1] http://dame.dsf.unina.it
[2] http://dame.dsf.unina.it/beta_info.html
[3] http://sci.esa.int/euclid/

2 Data Mining on massive data sets: An Overview

Let's start from a real and fundamental assumption: we live in a contemporary world submerged by a tsunami of data. Many kinds of data, tables, images, graphs, observed, simulated, calculated by statistics or acquired by different types of monitoring systems. The recent explosion of World Wide Web and other high performance resources of Information and Communication Technology (ICT) are rapidly contributing to the proliferation of such enormous information repositories. In all human disciplines, sciences, finance, societies, medicine, military, the archiving and electronic retrieval of data are by now both a common practice and the only efficient way to perform enterprises.

Despite of this situation, there is an important question: how are we able to handle, understand and use them in an efficient and complete way?

It is now widely recognized the chronic imbalance between growth of available data and ability to manage them (Hey et al. 2009).

In most cases the acquired data are not directly interpretable and understandable. Partially because they are obscured by redundant information or sources of noise, and mostly because they need to be cross correlated and in principle we never know

which is their hidden degree of correlation, also because in many cases we proceed to explore data without any prior knowledge about what we are looking for.

Moreover, for each social or scientific discipline the data are registered and archived in an inhomogeneous way, making inefficient the available tools useful to explore and correlate data coming from different sources.

Such a scenario imposes urgently the need to identify and apply uniform standards able to represent, archive, navigate and explore data in a homogeneous way, obtaining the required interoperability between the different disciplines.

This basic issue has been reflected within the recent definition (Hey et al. 2009) of the fourth paradigm of modern science, after theory, experiments and simulations. It is the E-science, which is the extraction of knowledge through the exploration of massive data archives, or Knowledge Discovery in Databases (KDD).

The fourth paradigm poses *in primis* the problem of the understanding of data, still before their representation or registering strategy. In scientific terms it implicitly identifies a methodology, based on the “with open mind” investigation and without any knowledge bias, of any kind of data set, in search of information useful to reveal the knowledge.

Of course this methodology imposes to make use of efficient and versatile computing tools, able to bridge the gap between human limited capacity (both in terms of processing time and 3D dimensionality) and progressive and steady growth in the quantity and complexity of the data. In other words able to replicate at a technological level the high learning, generalization and adaptation capabilities of human brain, by growing exponentially its information processing features.

These two prerogatives, investigation without knowledge bias and fast human intelligence, are not casually the milestones at the base of two rapidly growing disciplines: respectively Data Mining (DM) and Machine Learning (ML).

For those who prefer the formal definitions, DM can be easily defined as the extraction of information, implicit as well a priori unknown, from data.

But the definition of ML is not so easy to be formulated. There are in fact philosophical debates, partially divergent and hard to summarize in a single formal definition. However, in practice we can simplify its expression.

There are in particular two key concepts to be formally cleared: first, what we technically stand for learning? Second, how learning is practically connected to the machine (computer) processing rules?

Usually, in practical terms, what we can easily verify is not if a computer is able to learn, but mostly if it is able to give correct answers to specific questions. But such a level of ability is too weak to state that a computer has learned, especially if we consider that real learning is related to the generalization ability of a problem. In other words, to verify that a machine gives correct answers to direct questions, used to train it, is only the preliminary step of its complete learning. What is more interesting is the machine behavior in unpredicted situations, i.e. those never submitted to the machine during training.

Paraphrasing one of the key concepts of Darwinian theory of evolution of living species, ML is mainly interested to provide intelligence to a computer, i.e. adaptation and generalization to new or unpredicted evolving situations.

We defined above DM as the automatic or semi-automatic process of information discovery within massive data sets. After the previous considerations about ML, we are now able to provide an analogous operative definition also for it: a machine has learned if it is able to modify own behavior in an autonomous way such that it can obtain the best performance in terms of answer to external stimuli.

This definition shifts the focus on a different aspect of ML, which is not the pure knowledge but the adaptation performance in real and practical situations. In other words we are able to verify the training improvements through the direct comparison between present and past reaction performances. Indeed more in terms of evolution measurement rather than abstract knowledge.

But under theoretical aspects such kind of learning (evolution of behavior) is of course too much simple and weak. We know that also animals, considered less intelligent than humans, can be trained to evolve their reaction to external stimuli. But this does not necessarily mean that they have increased their knowledge, i.e. that they have really learned!

Learning is also thinking (*cogito ergo sum*, to cite the philosopher Descartes), which implies to have and use own cognitive properties to reach the goal. Not only to answer more or less in a right way to external stimuli. The latter is basically a passive process of action-reaction, not a real result of an active process of thinking and controlled behavior.

So far, the final role of ML must be more than evolution performance. To really decide if any machine was able to learn, it is inevitably needed to verify if the

machine may offer a conscious purpose and whether it is able to pursue and achieve its own abilities, acquired during training.

Besides these theoretical considerations, fortunately ML treats physical problems of real world, which are those composed or represented by tangible data and information, as result of direct or indirect observations/simulations. In such cases we can restrict the scope and interest of the ML and DM techniques, by focusing on their capability to identify and describe ordered structures of information within massive data sets (essentially structures in the data patterns), mixed with noise, together with the ability to predict the behavior of real complex systems. In other words, not only identification and prediction capabilities, but also description of the retrieved information, important for classification of unknown events.

2.1 A scientific use case: AstroInformatics

Over the last decade or two, due to the evolution of instruments and detectors, astronomy has become an immensely data rich science, thus triggering the birth of Astroinformatics: a new discipline placed at the crossroad between traditional astronomy, applied mathematics, computer science and ICT technologies. Among the other things, Astroinformatics aims at providing the astronomical community with a new generation of accurate and reliable methods and tools needed to reduce, analyze and understand massive and complex data sets and data flows which go far beyond the reach of traditionally used methods.

In the broadest sense, KDD/DM regards the discovery of “models” for data. There are, however, many different methods which can be used to discover these underlying models: statistical pattern recognition, machine learning, summarization,

etc., and an extensive review of all these models would take us far beyond the purposes of this paper. In what follows we shall therefore summarize only the main methodological aspects (Bishop 2006 and Duda 2001). Machine learning (ML), which is sometimes considered to be a branch of Artificial Intelligence (AI), is a scientific discipline concerned with the design and development of algorithms that allow computers to evolve behaviors based on empirical data. A "learner" can take advantage of examples (data) to capture characteristics of interest of their unknown underlying probability distribution.

These data form the so called Knowledge Base (KB): a sufficiently large set of examples to be used for training of the ML implementation, and to test its performance. The difficulty lies in the fact that often, if not always, the set of all possible behaviors given all possible inputs is too large to be covered by the KB. Hence the learner must possess some generalization capabilities in order to be able to produce useful output when presented new instances.

From a completely general point of view, regardless the specific method implemented, DM is a rather complex process. In most cases the optimal results can be found only on a trial and error base by comparing the outputs of different methods or of different implementations of the same method. This implies that in order to solve a specific problem a lengthy fine-tuning phase is often required. Such complexity is among the reasons for a slow uptake of these methods by the community of potential users which still fail to adopt them. In order to be effective, a DM application requires a good understanding of the mathematics underlying the methods, of the computing infrastructure, and of the complex workflows which need

to be implemented. So far, most domain experts in the scientific community are simply not willing to make the effort needed to understand the fine details of the process, and prefer to recur to traditional approaches which are far less powerful, but which may be more user-friendly. This situation is unsustainable as the ever larger MDS become available, and there will be no viable alternatives to DM methods for their exploration.

A good example of the challenges that have to be addressed by the astronomical community is the Large Synoptic Survey Telescope (LSST[4]) which should become operational within this decade, and which will produce a data flow of about 20 – 30 TB per observing night, or many PB/year. LSST raw data will therefore need to be calibrated, analyzed and processed in real time and, speed, accuracy and reliability become a must.

By addressing the case of space-based astronomical instrumentation, an important aspect involving machine learning is the data quality assessment: the so-called Data Quality Mining. A real case is the Euclid Mission spacecraft and detector (Brescia et al. 2011). As for a typical space observing instrument, sources and types of data outcoming from the Euclid system are:

1. Pre-mission data (catalogues, satellite and mission modeling data, etc.) used before and during the mission for calibration and modeling purposes mainly. The data for this processing level are prepared before the mission (and refined/updated during the in-flight commissioning and initial calibration phase) and are used as appropriate, before and during the mission.

[4] http://www.lsst.org/lsst/scibook

2. External data (images, catalogues, all relevant calibration and meta-data, observational data in science-usable format) derived from other missions and/or external survey projects, reformatted to be handled homogeneously with Euclid data. This data is required to allow the EC to provide its final data products at the expected level of accuracy. The data at this level is delivered by the EC.

3. Level 1: is composed of three separate processing levels, namely Level 1a, Level 1b and Level 1c.

    a. Level 1a refers to telemetry checking and handling, including real-time assessment (RTA) on housekeeping;

    b. Level 1b comprises quick-look analysis (QLA) on science telemetry, production of daily reports, trend analysis on instruments performance and production of weekly reports. The data for this processing level come from the satellite via MOC and are used to perform quality control.

    c. Level 1c refers to the high-quality removal of instruments signatures which provides data that will used to process Level 2 data.

4. Level 2: instrumental data processing, including the calibration of the data as well as the removal of instrumental features in the data. The data processing at this level is under the responsibility of the SDCs in charge of the instruments monitoring.

5. Level 3: data processing pipelines for the production of science-ready data. The Level 3 data are also produced by SDCs.

It goes without saying that the most valuable asset of Euclid are the data and, due to the huge data volume, the quality control becomes a crucial aspect of all five items

listed above and over the entire lifetime of the experiment: not only scientific data available at all various intermediate stages of the acquiring and processing workflows and pipelines, as it is foreseen during normal operations, but also telemetry, diagnostic, control, monitoring, calibration information coming in the ground segment from the instrument.

DM on MDS poses two important challenges for the computational infrastructure: asynchronous access and scalability.

Most available web-based DM services run synchronously, i.e., they execute jobs during a single HTTP transaction. This may be considered useful and simple, but it does not scale well when it is applied to long-run tasks. With synchronous operations, all the entities in the chain of command (client, workflow engine, broker, processing services) must remain up for the duration of the activity: if any component stops, the context of the activity is lost.

Regarding scalability, whenever there is a large quantity of data, there are three approaches to making learning feasible. The first one is trivial, consisting of applying the training scheme to a decimated data set. Obviously, in this case, the information may be easily lost and there is no guarantee that this loss is negligible in terms of correlation discovery. This approach, however, may turn very useful in the lengthy optimization procedure that is required by many ML methods (such as Neural Networks or Genetic Algorithms).

The second method relies in splitting the problem in smaller parts (parallelization) sending them to different CPUs and finally combine the results together. However, implementation of parallelized versions of learning algorithms is not always easy

(Rajaraman et al. 2010), and this approach should be followed only when the learning rule, such as in the case of Genetic Algorithms (Meng Joo et al. 2009), or Support Vector Machines (Chang et al. 2001), is intrinsically parallel. However, even after parallelization, the asymptotic time complexity of the algorithms cannot be improved.

A third and more challenging way to enable a learning paradigm to deal with MDS is to develop new algorithms of lower computational complexity, but in many cases this is simply not feasible (Paliouras 1993).

In some situations, background knowledge can make it possible to reduce the amount of data that needs to be processed by adopting a particular learning rule, since in many cases most of the measured attributes may turn out to be irrelevant or redundant when background knowledge is taken into account. In many exploration cases, however, such background knowledge simply does not exist, or it may introduce biases in the discovery process.

3 State of the art of computing technology

Over the years, the computational complexity of real-world problems and the scientific simulation completeness have increased hand in hand with available computational power. This chase to the performance has led to the need for a smarter management of available hardware resources and thus to create new architectures for High Performance Computing (HPC).

Actually the most important architectures commonly used are: Grid Computing, Cloud Computing and HPC.

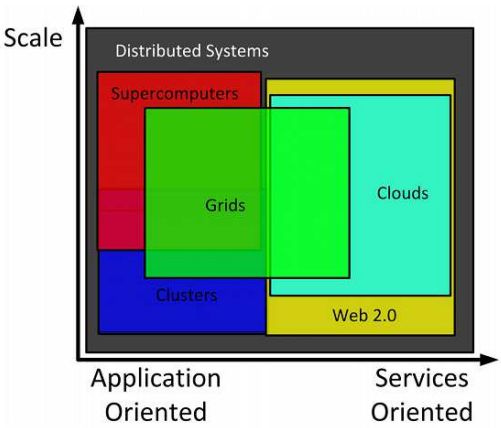


Figure 1 - Cluster-Grid-Cloud computing overview and comparison

3.1 GRID Computing

The term “the Grid” was coined in the mid-1990s to denote a (then) proposed distributed computing infrastructure for advanced science and engineering. Much progress has since been made on the construction of such an infrastructure and on its extension and application to commercial computing problems. And while the term “Grid” has also been on occasion applied to everything from advanced networking and computing clusters to artificial intelligence, there has also emerged a good understanding of the problems that Grid technologies address, as well as a first set of applications for which they are suited (Foster et al. 1998).

In a short time grid technologies have spread all over the world, especially in universities and research institutes due to the strong boost of the high energy physics experiments (such as CERN’s experiments) that involve large international collaborations.

The aim of grid computing is to share large amounts of memory and computing resources, distributed on a large scale, belonging to different administrative domains and characterized by a high degree of dynamism.

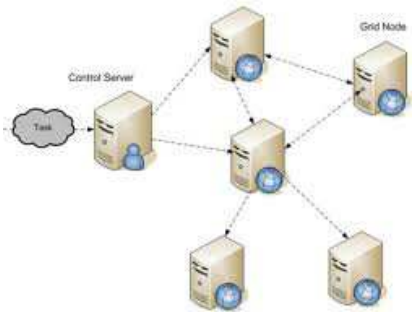


Figure 2 – Example of GRID architecture

This sharing is, necessarily, highly controlled, with resource providers and consumers defining clearly and carefully just what is shared, who is allowed to share, and the conditions under which sharing occurs. To deal the administration of this complex infrastructure, it introduces new important concepts and services compared to conventional distributed systems[5]

The first change brought, which is central to the philosophy of the Grid, is the concept of Virtual Organization (VOrg), which plays a key role, given the multi-disciplinary nature of large collaborations aimed at by this technology. A VOrg is defined as a set of mutually distrustful participants with varying degrees of prior relationship that want share resources in order to perform some task (Foster et al. 1998). It can also be composed of members of a single local institution, which shares the same structure with other campus (in case of campus Grid). Grid architectures are therefore designed to handle multi-VOrg environments that work together with different privileges and access policies about shared resources, unlike the traditional distributed systems.

Another important innovation of Grid systems is the high level of virtualization that mediates access to and virtualizes the hardware resource. One who logs the grid does not know the available resources and existing policies on them, so the access cannot be done with the classic login process.

The GRID introduces the concept of “GRID certificate” to authenticate users. A GRID certificate is issued by a Certificate Authority (CA) which checks the identity of the user and guarantees that the holder of this certificate exists and his certificate

[5] http://www.scope.unina.it/C8/grid-computing/default.aspx

is valid. The certificate is used for authentication instead of the user's account to avoid the replication of the user's account to all GRID sites. When authenticating to a site, the user's certificate is mapped to a local account under which all commands are executed. All GRID jobs use a proxy of the certificate with a limited lifetime. This enhances security because the user has to re-establish the validity of his certificate after the lifetime of the proxy has ended.

After logged in the user makes the discovering of available resources using community and integrated services according to the requirements of its applications. After an automatic or manual choice of the best resources, user's jobs are submitted from the front end to the physical Grid resources, which close the virtualization process, mapping the user on a local account that will run the applications. In Grid, a resource is a reusable entity that is employed to fulfill a job or resource request. It could be a machine, network, or some service that is synthesized using a combination of machines, networks, and software. The Resource broker is defined as an agent that controls the resource. It acts as a provider for a resource could provide the consumers with a ‘value added’ abstract resource (Krauter et al. 2002).

The scheduling is critical points of grid computing. Although this problem was extensively treated for several kinds of systems, many traditional approaches are inadequate to grid due its characteristics. While in traditional systems, resources and jobs are under the direct control of the scheduler, in Grids, the resources are heterogeneous, geographically distributed and belong to different individuals or organizations, each with their own scheduling policies, cost models of access, loads work and dynamic availability of resources through the time. The lack of centralized

control, along with the presence of users that generate jobs different from each other, make scheduling more complicated than in traditional computing systems. Due to the expensive scheduling decisions, data staging in and out, and potentially long queue times, many Grids don't natively support interactive applications.

3.2 CLOUD Computing

The name cloud computing was inspired by the cloud symbol that's often used to represent the Internet in flowcharts and diagrams.

Cloud computing means that the user applications and data are managed externally (online), rather than the user's machine (Viega 2009). The basic idea is to provide a heterogeneous collection of resources, where features are not known to the user. The main characteristic of cloud computing is to make available heterogeneous resources as if they were implemented by a single standard system. The actual implementation of the resources is not defined in detail as the architecture is service oriented.

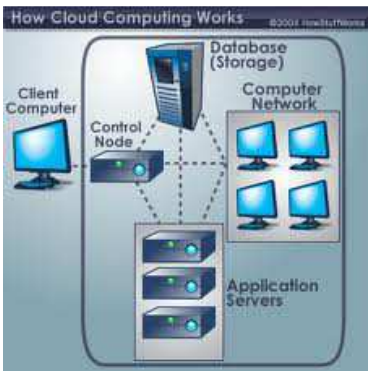


Figure 3 – Example of CLOUD architecture

A Cloud service has three distinct features that differentiate it from traditional hosting. It is sold on demand, typically by the minute or the hour; it is elastic, i.e. a user can have as much or as little of a service as he wants at any given time; and the service is fully managed by the provider. This "service provider hosting" fully handles the computer hardware and software architecture. Everything that the user needs is an Internet connection to access their data and to the applications for manage them. This approach allows access to facilities and services that are often cost-prohibitive for many organizations to meet or exceed.

These services are organized in three classes:

Software-as-a-Service (SaaS): In the SaaS model, the user buys a subscription to some software product, but some or all of the data and code resides remotely. It will be better than buying the hardware and software as keeps off the burden of updating the software to the latest version, licensing and is of course more economical. It doesn't keep any code on the client machine, even though some code might execute on the client temporarily. For example, Zoho Docs[6] (a Google alternative to Microsoft Office) relies on JavaScript, which runs in the Web browser. In this model, applications could run entirely on the network, with the user interface living on a thin client. In this layer, the users can access an application and information remotely via the Internet and pay only for that they use.

[6] https://www.zoho.com/docs/

Platform-as-a-Service (PaaS): From the consumer viewpoint, PaaS software probably resembles SaaS, but instead of software developers building the program to run on their own Web infrastructure, they build it to run on someone else's. PaaS offers an advanced integrated environment for building, testing, deploying and upgrading custom applications. For example, Microsoft offers Windows Azure[7], provides developers with on-demand compute, storage, networking and content delivery capabilities to host, scale and manages Web applications on the Internet through Microsoft data centers. A service that lets development organizations write programs to run specifically on Google's infrastructure.

Infrastructure-as-a-Service (IaaS): Similar to PaaS, IaaS lets the development organization to define its own software environment. This basically delivers virtual machine images to the IaaS provider, instead of programs, and the machines can contain whatever the developers want. The provider can automatically grow or shrink the number of virtual machines running at any given time so that programs can more easily scale to high workloads, saving money when resources aren't needed. The client typically pays on a *per-use* basis. Thus, clients can save cost as the payment is only based on how much resource they really use. Infrastructure can be expanded or shrunk dynamically as needed.

Cloud Computing model looks very different than Grid one, with resources in the Cloud being shared by all users at the same time (in contrast to dedicated resources

[7] https://partner.microsoft.com/italy/40084702

governed by a queuing system). This should allow latency sensitive applications to operate natively on Clouds, although ensuring a good enough level of QoS (Quality of Service) to the end users is not trivial, and it will likely be one of the major challenges for Cloud Computing as the Clouds grow in scale, and number of users (Foster et al. 2008).

3.3 High-Performance Computing (HPC)

The term is frequently used in the field of scientific calculus, generally referring to all technologies used to create processing systems capable of delivering very high performance of order of teraflop. The term is often used as a synonym for "supercomputer". In this case, the Clusters are a classical example of HPC, mainly used for calculations, rather than for I/O oriented operations like web services or database.

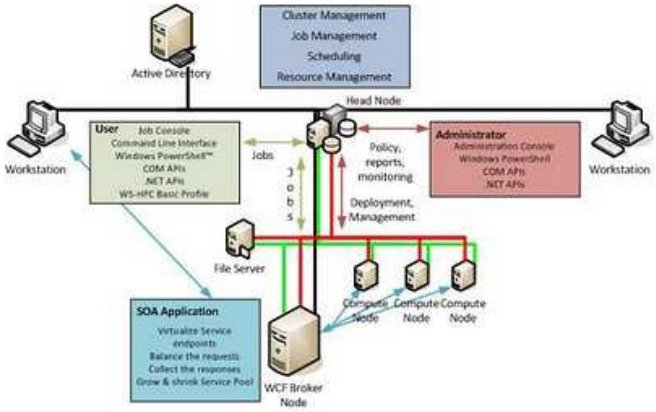


Figure 4 – Example of HPC architecture

HPC was once restricted to institutions that could afford the significantly expensive and dedicated supercomputers of the time. There was a need for HPC in small scale and at a lower cost which lead to cluster computing. The emergence of cluster platforms was driven by a number of academic projects, such as Beowulf[8] .

A Beowulf cluster (whose name is inspired by the eponymous hero of the epic Saxon) is a multi-computer architecture for parallel computing. Usually it consists of several client nodes controlled by a server node connected to each other via Ethernet. Once, they were created by assembling more homogeneous but less powerful PCs, creating bigger computing power. Beowulf was introduced in Astrophysics to do parallel processing of images observed by the CCD mosaic (mosaic detectors, where each CCD has a dedicated PC). Middleware systems such as MPI (Message Passing Interface) or PVM (Parallel Virtual Machine), allow the creation of clustering programs, portable across a wide variety of clusters.

HPC systems are used to solve advanced computational problems, for example: decoding genomes, animating movies, analyzing financial risks, streamlining crash test simulations, modeling global climate solutions and other highly complex problems, always characterized by extreme processing complexity. The most common way of solving complex problems has been to use specialized supercomputing hardware, leading to increase the costs to purchase new hardware, which would become obsolete quickly.

[8] http://www.beowulf.org/

3.4 GPGPU

GPGPU is an acronym standing for General Purpose Computing on Graphics Processing Units. It was invented by Mark Harris in 2002 (Harris 2003), by recognizing the trend to employ GPU technology for not graphic applications.

With such term we mean all techniques able to develop algorithms extending computer graphics but running on graphic chips. Up to 2006 these chips have been difficult to be used, mainly because programmers were conditioned to use specific APIs (Application Programming Interface) to access to graphic devices, hence based on methods made available by libraries like OpenGL and Direct3D. These APIs often were strongly limiting applications design and development.

In general the graphic chips, due to their intrinsic nature of multi-core processors (many-core) and being based on hundreds of floating-point specialized processing units, make many algorithms able to obtain higher (one or two orders of magnitude) performances than usual CPUs (Central Processing Units). They are also cheaper, due to the relatively low price of graphic chip components.

Particularly useful for super-computing applications, often requiring several execution days on large computing clusters, the GPGPU paradigm may drastically decrease execution times, by promoting research in a large variety of scientific and social fields (such as, for instance, astrophysics, biology, chemistry, physics, finance, video encoding and so on).

Besides the architecture intrinsically compliant with parallel computing, since the 2007 there was an increasing of programming tools, offered by commercial solutions, growing the computing power and availability. This evolution is still

extending its exploit, also due to the recent upgrade of the 3D technology (in most cases pushed up by videogames world). In the past the video technology was based on a pipeline of pre-defined and static instructions, but progressively it started to evolve towards a new approach, in which the GPUs are fully programmed by using the shader models. In the field of computer graphics, a shader is a set of software instructions that is used primarily to calculate rendering effects on graphics hardware with a high degree of flexibility. Shaders are used to program the GPUs programmable rendering pipeline, which has mostly superseded the fixed-function pipeline that allowed only common geometry transformation and pixel-shading functions; with shaders, customized effects can be used (Ebert et al. 2000).

Nowadays there is available the shader model 4.0, also named as "model with unified shaders", able to use the same instruction set to handle different types of shaders. This solution can optimize the dynamical resource management for different types of shaders. More in detail, while past GPU generations were simply devices able to extend classical graphic pipeline, last generation GPUs have a more flexible internal engine, supported by a series of processing units specialized in a predetermined function (Owens et al. 2008).

3.5 A discussion about computing architectures

For over two decades, before the advent of multi-core architectures, the general purpose CPUs have been characterized, at each generation, by an almost linear increasing of performances together with a decreasing of costs, also known as Moore's Law (Moore 1965), shown in Figure 5,

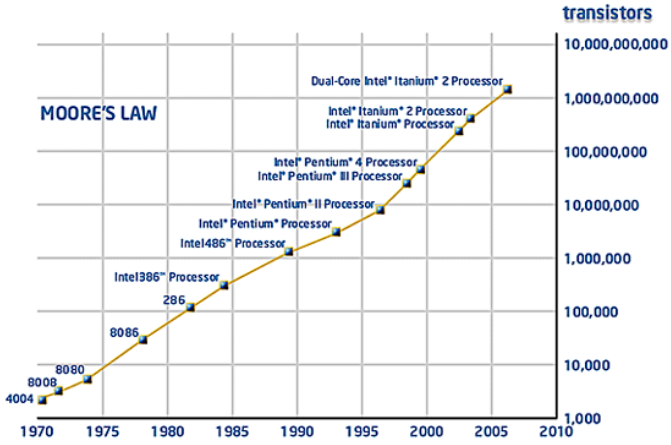


Figure 5 – The Moore's CPU Law

So far, we have now available low-cost desktop PCs able to execute tens of Giga floating-point Operations per Second (GFLOPS) and server clusters with hundreds of GFLOPS.

This performance growth engaged a fundamental virtuous cycle in the Computer Science:

- Users, being rapidly used to performance growth for computers, especially in terms of execution speed, processing reliability and multi-tasking capability, are continuously asking for better software systems;

- Developers, by observing the constant increase of software performances, together with processor technology, always ask for better hardware performances to optimize application speed.

There is a downside of this virtuous mechanism. The physical constraints of Thermodynamics started to cause relevant problems of power consumption and heat

dissipation inside the modern CPUs, by slowing such evolution trend and by forcing computer manufacturers to a drastic revolution in the processor architecture design. In fact, in order to make feasible this linear trend of performances, by controlling the thermal effects, the new strategy was to reduce the clock frequencies and to distribute working loads over several processing units (cores) located on the same chip. From the architectural point of view, such new roadmap has inevitably changed the design approach adopted up to now in the software development environment.

They in fact moved away from the past sequential structure. Such methodology appeared obsolete on the new multi-core infrastructure, essentially because the sequential program can run on a single core, leaving unexploited the rest of processor cores.

Furthermore, without an effective growth of performances, the developers would not be able to introduce new features in the software products, blocking de facto the evolution of the entire computer science business.

So far, in order to maintain the cyclic hardware/software trend, the software applications had to change their perspective, moving towards parallel computing, able to fully exploit the availability of parallel architectures. The first systems, on which the parallel programming started, were indeed HPC mainframes.

However they are machines, or infrastructures in the Grid/Cloud cases, having some critical points:

- Large dimensions;
- High costs for equipment and management;
- Difficult to be accessed by external developers and users;

With such problems, many applications are not able to justify these high costs and this was hardly limiting in practice the parallel programming dissemination.

Nowadays the multi-core technology has reached so high sales volumes that a parallel programming approach can be considered as usual. This caused a trend inversion in the software development field.

At the beginning of 2000 every silicon farm posed an important question: which roadmap to follow in the processor development to reach the business goals?

Multi-core processors were selected by many companies, such as, for instance, Advanced Micro Devices Inc. (AMD), ARM Ltd., Broadcom Corp., Intel Corp. e VIA Technologies. Examples of last generation multi-core architectures are present either in the AMD Phenom X4 and Intel Core i7 families.

More specifically, these multi-core processors are based on an integrated circuit in which two or more processors were connected to the same socket, in order to increase their connection speed. Each core implements the full set of x86 instructions and it enhances the performances, reduces consumptions and implements a more efficient multi-tasking. First models were dual-core, comparable

to dual-processor systems. Ideally indeed, a dual-core processor would be about two times more powerful of a single-core processor. But in practice this gap is about one and half times.

The evolution of such architecture proceeds through a slow enhancement, in which the number of cores doubles with every new semi-conductor generation. The basic idea is to grow the core number by maintaining unchanged the execution speed of pre-existent sequential programs.

The critical points for such architecture come out in case of serial programs. In this case, in the absence of the parallel approach, the processes are scheduled in such a way that the full load on the CPU is balanced, by distributing them over the less busy cores each time. However many software products are not designed to fully exploit the multi-core features, so far the micro-processors are designed to optimize the execution speed on sequential programs.

The choice of graphic device manufacturers, like ATI Technologies Inc. (acquired by AMD in the 2006) and NVIDIA Corp., was the many-core technology (usually many-core is intended for multi-core systems over 32 cores). The many-core paradigm is based on the growth of execution speed for parallel applications. Began with tens of cores smaller than CPU ones, such kind of architectures reached hundreds of core per chip in a few years.

An example of many-core architecture is the graphic device NVIDIA GeForce GTX 560, with 336 cores, also named Streaming Processor (SP). These cores are grouped into units, called Streaming Multiprocessor (SM), of 8 cores each (hence in our case

336/8 = 42 SM). Each SP is an in-order executed scalar processor and it shares both control logic and instruction cache with others.

The many-core processors, in particular GPU, have led the race for floating point computation performance since 2004, as shown in Figure 6 (Kirk et al 2010).

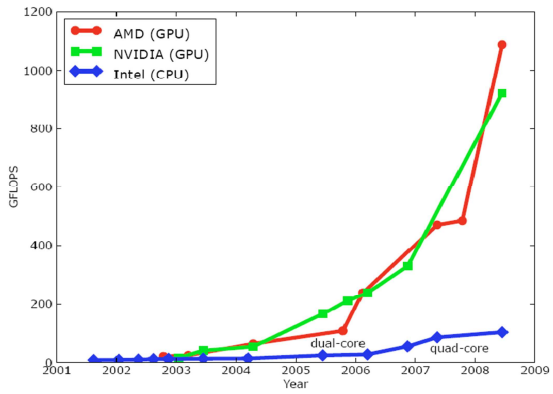


Figure 6 – CPU vs. GPU throughput evolution

Since 2009 the throughput peak ratio between GPU (many-core) and CPU (multi-core) was about 10:1. It must be issued that such values are referred mainly to the theoretical speed supported by such chips, i.e. 1 TeraFLOPS against 100 GFLOPS.

Such a large difference has pushed many developers to shift more computing-expensive parts of their programs on the GPUs. The large difference between GPU and CPU is basically located into the different design philosophy, as shown in Figure 7[9].

[9] http://developer.nvidia.com/nvidia-gpu-computing-documentation

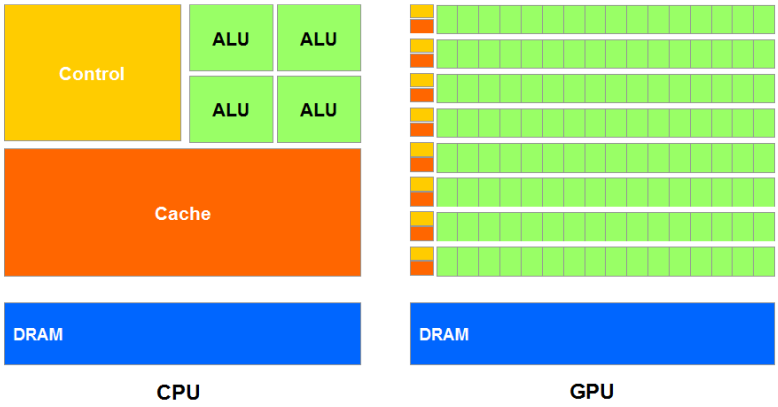


Figure 7 – CPUs and GPUs different design philosophies.

In order to maximize the efficiency of sequential code, the CPU must be designed by following some constraints:

- sophisticated control logics, in order to make single process instructions able to be executed in parallel (pipelining and multi-threading) or without to follow the execution order imposed by the programmer (out-of order execution), by appearing as sequentially executed;

- cache memories of large dimensions, in order to reduce the latency time during data access or complex instruction execution;

- high difference of memory bandwidth between CPU and graphic chips (about ten times higher), due to the requirements (coming from operative systems, applications and I/O devices), to be satisfied by general-purpose processors. This makes difficult a growth of memory bandwidth. On the contrary, by having more simple memory models and fewer constraints to follow, GPU designers have been able to enhance the memory bandwidth in a more easy way. For instance, the chip NVIDIA GTX 590 has

a memory bandwidth of about 328 GB/sec, while an Intel Core i7-2600 reaches only 20 GB/sec.

Videogames have mainly led and caused such technical evolution trend all over these years. The demand of higher performances at low cost, together with the need to obtain a higher number of floating point calculations in less time, caused the optimization of throughput in the GPUs for the multi-threading execution. Such hardware is able to exploit the entire GPU at all processing time, by also reducing the control logic needed for each execution process. In order to maximize the number of threads accessing to same data in memory, without having to access to the DRAM, several smaller cache memories are used, helping to respect the bandwidth requirements. This results in a larger area than chip addressable by floating point calculations.

The GPUs are particularly efficient to solve problems with a strongly parallel structure of data. Being able to execute same instructions over each data-element, there are less strong requirements about control logic.
The latency time of memory access can be masked by the execution time, instead of using larger cache memories.
However the GPUs provide high performances on specific cases only: scientific calculations, parallel computing and massive data sets navigation. So far, the applications which want to exploit all their features will have to use GPUs for more complex computations, by devoting CPUs for the rest of the sequential code.

It is important to point out that the performances are not the unique decisional factor whenever processors are to be selected for specific applications. Other important factors could also be:

- Standards to follow: such as IEEE (Institute of Electrical and Electronics Engineers) 754, for floating point calculation[10]. In general to follow specific standards has the advantage to obtain reproducible results with different processors. GPUs, starting to support single-precision floating point calculation, have reached a level comparable with CPU with double-precision. We expect indeed to extend the scientific application range running on GPUs;

- A wide presence on the marketplace of the particular processor category, in order to justify the software development costs through a large user base. By using processors with a low distribution it may cause a low use of the technology. This was the case in the past for parallel computing. But as said before, this situation has been changed by the introduction of GPGPU technology.

In conclusion, we are living a particular dynamical era, in which the proliferation of different computing paradigms reflect the recent recognition of e-science as the fourth leg of Science, after theory, experimentation and simulation. All these computing architectures have pro and cons, summarized in the following table.

[10] IEEE Standard for Floating-Point Arithmetic
http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=4610935

In the following Table 1 (Sadashiv et al. 2011), we summarize a comparison between Cluster, Grid and Cloud Computing paradigms. GPGPU can be only partially involved in that comparison, because specifically dedicated to parallel computing.

FEATURE	CLUSTERs	GRIDs	CLOUDs
Service Level Agreement	limited	yes	Yes
Allocation	centralized	decentralized	Both
Resource Handling	centralized	distributed	Both
Loose coupling	no	both	Yes
Protocols/API	MPI, parallel virtual	MPI, MPICH-G, GIS, GRAM	TCP/IP, SOAP, REST, AJAX
Reliability	no	half	Full
Security	yes	half	No
User friendliness	no	half	Yes
Virtualization	half	half	Yes
Interoperability	Yes	yes	Half
Standardized	yes	yes	No
Business Model	no	no	Yes
Task Size	Single large	Single large	Small & medium
SOA	no	yes	Yes
Multi tenancy	no	yes	Yes
System Performance	improves	improves	Improves
Self service	no	yes	Yes
Computation service	computing	Max. computing	On demand
Heterogeneity	no	yes	Yes
Scalable	no	half	Yes
Inexpensive	no	no	Yes
Data Locality exploited	no	no	Yes
Application	HPC, HTC	HPC, HTC, Batch	SME interactive apps
Switching cost	low	low	High
Value added service	no	half	Yes

Table 1 – Cluster, Grid and HPC comparison

3.6 Parallel programming environment

3.6.1 Conventional programming environment: MPI and OpenMP

Parallel programming environments provide the basic tools, language features and programming interfaces (APIs) needed to build a parallel program. This programming environment uses an abstraction called a programming model. The sequential computers use the well-known model of von Neumann (von Neumann 1945). Because all sequential computers use this model, developers who program in this software abstraction can map onto most, if not all, sequential computers. Otherwise, there are many possible models for parallel computing.

Due to the wide range of parallel architectures, the research of programmers has been historically focused on hundreds of parallel programming environments.

Fortunately, by the late 1990s, the parallel programming community converged predominantly on two environments for parallel programming: Message Passing Interface (MPI) for the scalable cluster calculations (i.e. distributed memory systems) and OpenMP for multi-processor systems with shared memory (Mattson et al. 2004).

MPI is a model in which the computing nodes of a cluster do not share memory[11]. Both data sharing and interactions occur through an explicit message exchange. MPI has been much more employed in the scientific high performance computing domain. There are in fact, known MPI applications able to work on cluster systems with more than 100.000 nodes. However the huge effort for the porting of an

[11] http://www.mpi-forum.org/docs/-2.2/-report.pdf

application on this infrastructure could be extremely expensive, especially in case of absence of shared memory between computing nodes.

On the contrary, OpenMP is quite simple to be programmed. Main advantages come out from the fact that there are APIs handled by issues from the specific compiler used (for example, the C code fragment reported below): easier programming, incremental parallelism (i.e. it is possible to work on a code portion at a time without drastic changes to the serial code) and unified applications with parallel and serial code (because the OpenMP blocks are considered as comments by sequential compilers). However there is the risk to introduce bugs due to synchronization errors[12]. Anyway, with such APIs it is not possible to reach scalability higher than two hundred computing nodes, because there are strict hardware requirements concerning the overhead of thread handling and cache coherency.

```
int main(int argc, char *argv[]) {
   const int N = 100000;
   int i, a[N];

 #pragma omp parallel for
   for (i = 0; i < N; i++)
       a[i] = 2 * i;

   return 0;
}
```

Listing 1 - Example of OpenMP Pragma

[12] http://developers.sun.com/solaris/articles/cpp_race.html

3.7 GPGPU environment: CUDA

CUDA (Compute Unified Device Architecture) is a general purpose parallel computing architecture introduced by NVIDIA in November 2006 that leverages the parallel compute engine in NVIDIA GPUs to solve many complex computational problems in a more efficient way than on a CPU. It includes the CUDA Instruction Set Architecture (ISA) and the parallel compute engine in the GPU.

CUDA comes with a software environment that allows developers to use C as a high-level programming language. Other languages or API are supported, such as CUDA FORTRAN, OpenCL, and DirectCompute.

To the hardware perspective, NVIDIA devoted silicon area to facilitate the ease of parallel programming, so this did not represent a change in software alone; additional hardware was added to the chip. CUDA programs no longer go through the graphics interface at all. Instead, a new general-purpose parallel programming interface on the silicon chip serves the requests of CUDA programs.

3.7.1 CUDA architecture

Unlike previous generations that partitioned computing resources into vertex and pixel shaders, the CUDA Architecture included a unified shader pipeline, allowing each and every arithmetic logic unit (ALU) on the chip to be marshaled by a program intending to perform general-purpose computations. Because NVIDIA intended this new family of graphics processors to be used for general-purpose computing, these ALUs were built to comply with IEEE requirements for single-

precision floating-point arithmetic and were designed to use an instruction set tailored for general computation rather than specifically for graphics.

Furthermore, the execution units on the GPU were allowed arbitrary read/write access to memory as well as access to a software-managed cache known as shared memory. All of these features of the CUDA Architecture were added in order to create a GPU that would excel at computation in addition to performing well at traditional graphics tasks.

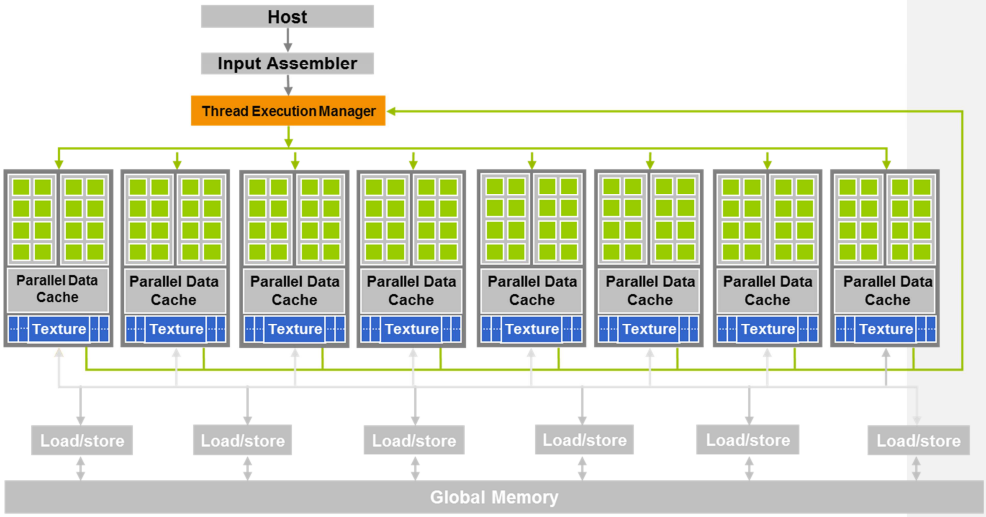


Figure 8 - CUDA GPU Architecture

A typical CUDA-capable GPU is organized into an array of highly threaded streaming multiprocessors (SMs).

In Figure 8, two SMs form a building block; however, the number of SMs in a building block can vary from one generation of CUDA GPUs to another generation. Also, each SM has a number of streaming processors (SPs) that share control logic

and instruction cache. Each GPU currently comes with up to 4 GB of graphics double data rate (GDDR) DRAM, referred to as global memory. They function as very-high-bandwidth, off-chip memory, though with somewhat more latency than typical system memory. For massively parallel applications, the higher bandwidth makes up for the longer latency. Each SP has a multiply–add (MAD) unit and an additional multiply unit. In addition, special-function units perform floating-point functions such as square root (SQRT), as well as transcendental functions. Because each SP is massively threaded, it can run thousands of threads per application.

3.7.2 Memory Hierarchy

In CUDA, the host and devices have separate memory spaces. CUDA threads may access data from multiple memory spaces during their execution as illustrated by Figure. Each thread has private local memory. Each thread block has shared memory visible to all threads of the block and with the same lifetime as the block. All threads have access to the same global memory. At the bottom of the figure, we see global memory and constant memory that allows read-only access by the device code. These are the memories that the host code can transfer data to and from the device, as illustrated by the bidirectional arrows between these memories and the host.

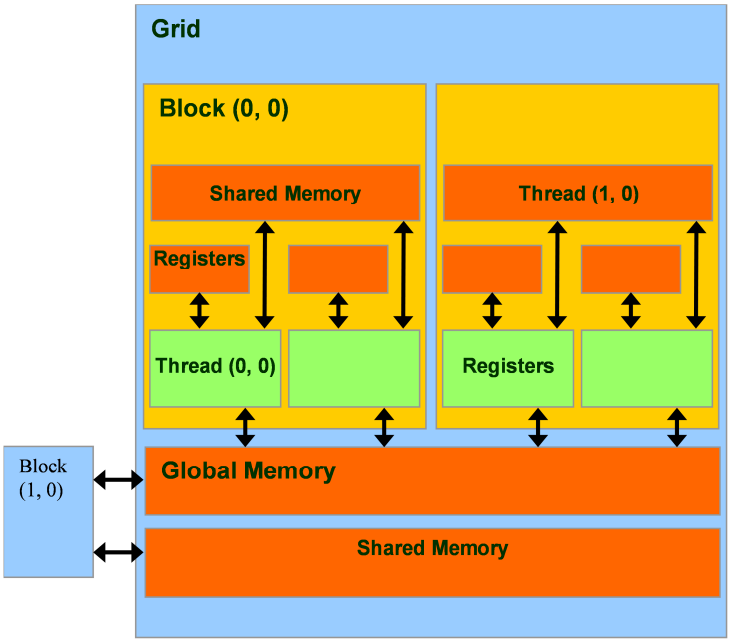


Figure 9 - Overview of the CUDA memory model

3.7.3 Thread Hierarchy

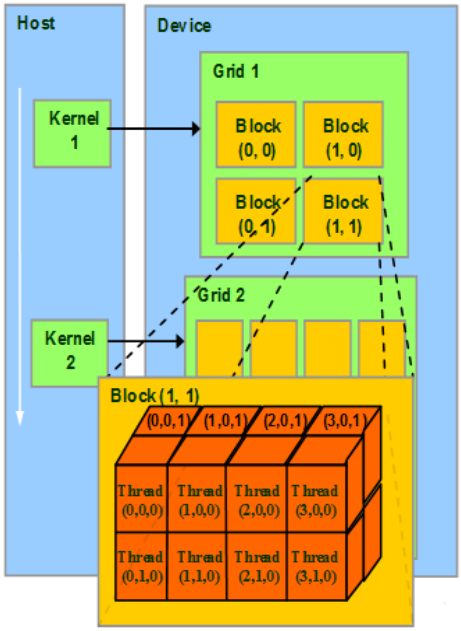


Figure 10 - CUDA thread organization

When a kernel is invoked, it is executed as grid of parallel threads. Each CUDA thread grid typically is comprised of thousands to millions of lightweight GPU threads per kernel invocation. For simplicity, a small number of threads are shown in Figure 10.

Threads in a grid are organized into a two-level hierarchy, where at the top level, each grid consists of one or more thread blocks. All blocks in a grid have the same number of threads. Each block has a unique two-dimensional coordinate given by

the CUDA specific keywords blockIdx.x and blockIdx.y. All thread blocks must have the same number of threads organized in the same manner. Blocks are organized into a one-dimensional, two-dimensional, or three-dimensional array of threads. On current GPUs a thread block may contain up to 1024 threads. Threads with the same threadIdx values from different blocks would end up accessing the same input and output data elements. When the host code invokes a kernel, it sets the grid and thread block dimensions via execution configuration parameters.

3.7.4 CUDA C Parallel Programming Model

The introduction of multicore CPUs and manycore GPUs introduced the challenge is to develop application software that transparently scales its parallelism to leverage the increasing number of processor cores.

The CUDA parallel programming model is designed to overcome this challenge while maintaining a low learning curve for programmers familiar with standard programming languages such as C.

At its core are three key abstractions: a hierarchy of thread groups, shared memories, and barrier synchronization.

These abstractions provide fine-grained data parallelism and thread parallelism, nested within coarse-grained data parallelism and task parallelism. They guide the programmer to partition the problem into coarse sub-problems that can be solved independently in parallel by blocks of threads, and each sub-problem into finer pieces that can be solved cooperatively in parallel by all threads within the block.

This decomposition preserves language expressivity by allowing threads to cooperate when solving each sub-problem, and at the same time enables automatic scalability. Indeed, each block of threads can be scheduled on any of the available processor cores, in any order, concurrently or sequentially, so that a compiled CUDA program can execute on any number of processor cores as illustrated by Figure 9, and only the runtime system needs to know the physical processor count.

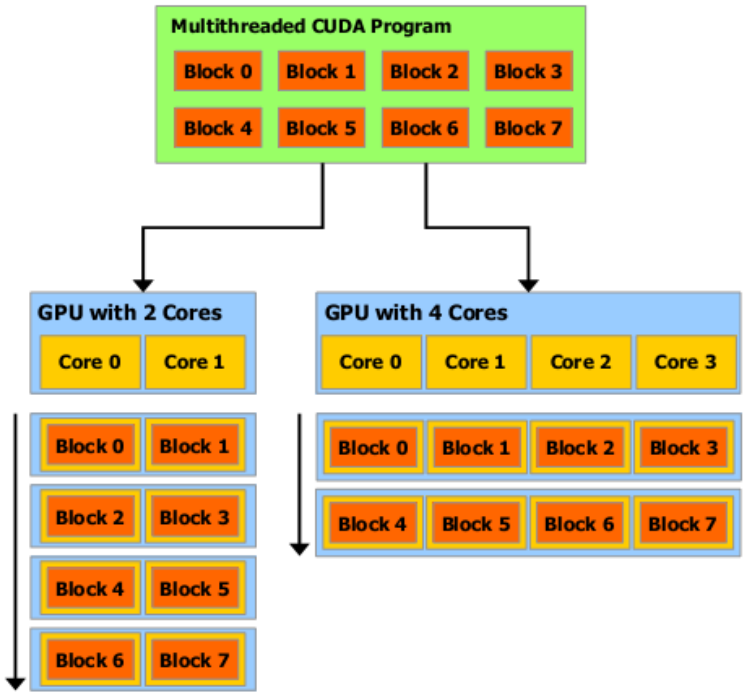


Figure 11 – CUDA with different multi-core architectures

This scalable programming model is designed for transparent and portable scalability. It allows the CUDA architecture to span a wide market range, from the high-performance Tesla GPUs to the inexpensive mainstream GeForce GPUs, by

scaling the number of processors and memory partitions. A CUDA program is written once and runs on a GPU with any number of processor cores.

3.7.5 CUDA Program Structure

A CUDA program consists of one or more phases that are executed on either the host (CPU) or a device such as a GPU. The phases that exhibit little or no data parallelism are implemented in host code. The phases that exhibit rich amount of data parallelism are implemented in the device code.

A CUDA program is a unified source code encompassing both host and device code. While the host code is straight ANSI C code, the device code is written using ANSI C extended with keywords for labeling data-parallel functions, called *kernels*, and their associated data structures. The kernels typically generate a large number of threads to exploit data parallelism. Due to efficient hardware support the CUDA threads are of much fast and lighter weight than the CPU threads that typically require thousands of clock cycles to generate and schedule.

The execution of a typical CUDA program starts with host (CPU) execution. When a kernel function is invoked, the execution is moved to a device (GPU), where a large number of threads are generated to take advantage of abundant data parallelism. All the threads that are generated by a kernel during an invocation are collectively called a grid. When all threads of a kernel complete their execution, the corresponding grid terminates, and the execution continues on the host until another kernel is invoked.

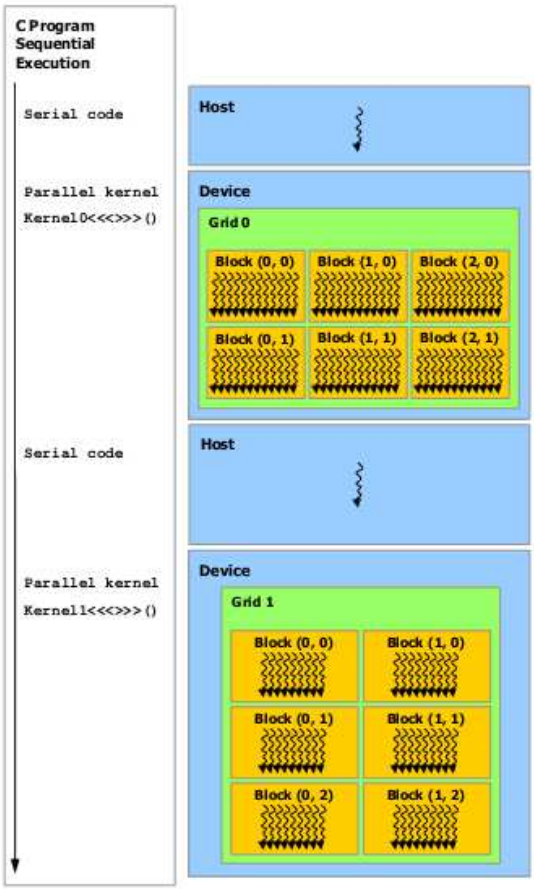


Figure 12 - CUDA program structure

3.7.6 Other GPGPU environment: OpenCL

Recently, some collaboration between major industries, including Apple, Intel, AMD (formerly ATI) and NVIDIA developed a programming model for development on heterogeneous architectures across CPU, GPU and other types of processors, called OpenCL (Open Computing Language). OpenCL will form the

foundation layer of a parallel computing ecosystem of platform-independent tools, middleware and applications.

OpenCL has been proposed as an open standard. Similar to CUDA, OpenCL programming model defines a language, based on the C99 programming language with extensions and restrictions, and runtime APIs to allow programmers the management of data parallelism and massively parallel processors[13].

OpenCL, being a standardized programming model, allows all applications, requiring to be developed in this language, to be executed without any modification to the code, on all devices that support language extensions and APIs.

OpenCL is a technology less known than CUDA. Its level of programming rules is still less advanced than in CUDA and it is more complex to be used, due to the absence of a unified SDK (Software Development Kit) to be shared among all manufacturers.

Furthermore, on the platforms supporting both technologies, the speed reached by OpenCL applications is still less than CUDA, an important factor influencing developers, always demanding higher processing speed.

For completeness, we mention the development environments created by ATI: CTM (Close To Metal) and Stream. These two programming models have been early abandoned in favor of OpenCL, whose basic positive and negative features can be summarized as follows:

[13] http://www.khronos.org/registry/cl/sdk/1.0/docs/man/xhtml/

Pros

- Acceleration in parallel processing;
- It allows to manage computational resources
  - View multi-core CPUs, GPUs, etc. as computational units;
  - Allocate different levels of memory;
- Cross-vendor software portability
  - Separation of low-level and high-level software;
- Much wider range of hardware and platform support;
  - Supports AMD, NVIDIA and Intel GPUs equally. It can also be used on newer versions of Android phones, iPhones and other devices;
- It can fallback on CPU if the GPU support does not exist;
  - In reality, to create thousands of threads on the CPU, it is generally not a good idea;
- Supports synchronization over multiple devices;
- Easy to get started with integrating OpenCL kernels in to the code.
- An open standard and not vendor locked and a kernel language based on C99 specification.

Con

- public drivers to support OpenCL 1.1. Currently only developer ones exist;
- Lacks mature libraries;
- Debugging and profiling tools are not as advanced as CUDAs.

Moreover, the following table reports a direct comparison between OpenCL and CUDA (Rosendahl 2010).

FEATURE	CUDA	OpenCL
What it is	HW architecture, ISA, API, programming language, SDK and tools	Open API and language specification
Proprietary or open technology	Proprietary	Open and royalty-free
When introduced	Q4 2006	Q4 2008
Free SDK	Yes	Depends on vendor
OS support	Windows, Linux, Mac OS X;	Depends on vendor
Heterogeneous device support	No, just NVIDIA GPUs	Yes (CPUs and GPUs)
Development models compared		
Multiple kernel programming languages	Yes	No, possible vendor-specific language
Multiple programming interfaces	Yes, including OpenCL	No, possible vendor extensions
Data parallel kernels support	Yes, the default model	Yes
Task parallel kernels support	No, at least not efficiently	Yes
Device level language	Yes, PTX	Implementation specific or no intermediate language used
Deep host and device program integration	Yes, with syntax calls	No, only separate compilation
Kernel programming differences		
Base language version defined	"Based on C", limited C++ features are supported	C99
Access to work-item indices	Through built-in variables	Through built-in functions
Address space qualification needed for kernel pointer arguments	No, defaults to global memory	Yes
First-class built-in vector types	Vector types	Vector types, literals, built-in operators and functions
Voting functions	Yes (CC 1.2 or greater)	No
Atomic functions	Yes (CC 1.1 or greater)	Only as extension
Asynchronous memory copying and pre-fetch functions	No	Yes
Support for C++ language features	Yes, useful subset of features supported	Experimental interface

Table 2 – CUDA vs. OpenCL comparison

4 Technology in machine learning

The sheer size of the foreseen data streams renders impossible to discriminate objects using traditional software tools, and requires the development of specific computing infrastructures as well as the implementation of specific and robust (largely based on the ML paradigm) methods for data analysis and understanding. ML methods, in order to provide efficient and reliable answers, need also to exploit all the meta-information made available to any scientific/social community through the data repositories federated under specific data centers or virtual organizations (Genova et al. 2002).

The problem of inventing and deploying these new tools under powerful computational infrastructure has therefore become a worldwide challenge. On the algorithmic side, we wish to emphasize that commonly used decision algorithms depend on a fixed number of predefined input features for decision making. This is not the best option in Time Domain Analysis where some of the inputs may not be present within the time slot available to make the decision.

There is therefore a demand for a completely new class of tools that can dynamically select the input features and can consistently give reliable predictions. Most decision algorithms compute the inverse Bayesian probability to deal with missing attributes (mostly called features) in the input data.

Although such algorithms can handle missing features to some extent, there is always a possibility for asymptotic decline in accuracy. It may be argued that the possible state of the missing feature can be adequately constrained and compensated for by the available remaining inputs.

However this is not true, because a feature that can be well constrained by the remaining inputs is usually redundant and it is not required as an input at the first place. If this is not the case, its absence can't be appropriately compensated and that will result in a loss of information.

The idea therefore is to facilitate dynamic learning in which, for instance, the system learns from all available information (and not on a fixed set of samples) and identify strategies that can optimally handle situations in which most of the inputs are missing.

As already underlined, one of next main breakthroughs in many human fields is that we have reached the physical limit of observations. So far, like all scientific disciplines focusing their discoveries on collected data exploration, there is a strong need to employ e-science methodology and tools in order to gain new insights on the knowledge. But this mainly depend on the capability to recognize patterns or trends in the parameter space (i.e. physical laws), possibly by overcoming the human limit of 3D brain vision, and to use known patterns as Base of Knowledge (BoK) to infer knowledge on self-adaptive models in order to make them able to generalize feature correlations and to gain new discoveries (for example outliers identification) through the unbiased exploration of new collected data. These requirements are perfectly matching the paradigm of ML techniques based on the Artificial Intelligence

postulate (Bishop 2006). Hence, in principle at all steps of an exploration workflow ML rules can be applied. Let us better know this methodology.

There is a basic dichotomy in ML, by distinguish between supervised and unsupervised methodology, as described in the following.

The Greek philosopher Aristotle was one of the first to attempt to codify "right thinking," that syllogism is, irrefutable reasoning processes. His syllogisms provided patterns for argument structures that always yielded correct conclusions when given correct premises. For example, "Socrates is a man; all men are mortal; therefore, Socrates is mortal." These laws of thought were logic supposed to govern the operation of the mind; their study initiated the field called logic**.** Logicians in the 19th century developed a precise notation for statements about all kinds of things in the world and about the relations among them. Contrast this with ordinary arithmetic notation, which provides mainly for equality and inequality statements about numbers.

By 1965, programs existed that could, in principle, process any solvable problem described in logical notation (Moore 1965). The so-called logicist tradition within artificial intelligence hopes to build on such programs to create intelligent systems and the ML theory represents their demonstration discipline. Reinforcement in this direction came out by integrating ML paradigm with statistical principles following the Darwin's Nature evolution laws, (Duda et al. 2001).

4.1 The learning paradigms

In supervised ML we have a set of data points or observations for which we know the desired output, expressed in terms of categorical classes, numerical or logical variables or as generic observed description of any real problem. The desired output is in fact providing some level of supervision in that it is used by the learning model to adjust parameters or make decisions allowing it to predict correct output for new data. Finally, when the algorithm is able to correctly predict observations we define it a classifier. Some classifiers are also capable of providing results in a more probabilistic sense, i.e. a probability of a data point belonging to class. We usually refer to such model behavior as regression.

A typical workflow for supervised learning is shown in the diagram below (Figure 13).

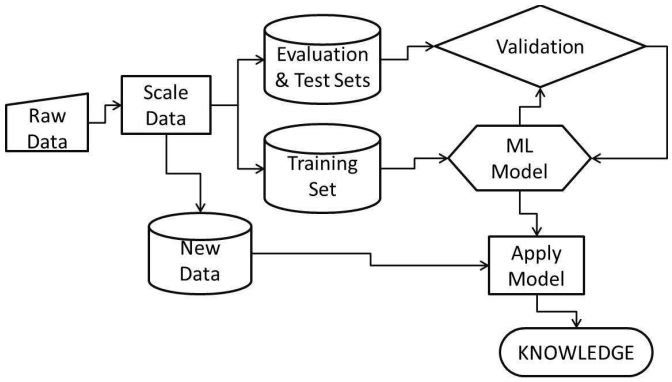


Figure 13 – A workflow based on supervised learning paradigm

The process is:

- *Pre-processing of data*. First we need to build input patterns that are appropriate for feeding into our supervised learning algorithm. This includes scaling and preparation of data;

- *Create data sets for training and evaluation.* This is done by randomly splitting the universe of data patterns. The training set is made of the data used by the classifier to learn their internal feature correlations, whereas the evaluation set is used to validate the already trained model in order to get an error rate (or other validation measures) that can help to identify the performance and accuracy of the classifier. Typically you will use more training data than validation data;

- *Training of the model*. We execute the model on the training data set. The output result consists of a model that (in the successful case) has learned how to predict the outcome when new unknown data are submitted;

- *Validation*. After we have created the model, it is of course required a test of its performance accuracy, completeness and contamination (or its dual, the purity). It is particularly crucial to do this on data that the model has not seen yet. This is main reason why on previous steps we separated the data set into training patterns and a subset of the data not used for training. We intend to verify and measure the generalization capabilities of the model. It is very easy to learn every single combination of input vectors and their mappings to the output as observed on the training data, and we can achieve a very low error in doing that, but how does the very same rules or mappings perform on new data that may have different input to output mappings? If the classification error of the validation set is higher than the training error, then we have to go back and adjust model parameters. The reason could be that the model has essentially memorized the answers seen in the training data, failing its generalization capabilities. This is a typical behavior in case of overfitting, and there are various techniques for overcoming it;

- Use. If validation was successful the model has correctly learned the underlying real problem. So far we can proceed to use the model to classify/predict new data.

The kinds of problems that are suited for unsupervised algorithms may seem similar, but are very different to supervised learners. Instead of trying to predict a set of known classes, we are trying to identify the patterns inherent in the data that separate like observations in one way or another. In other words, the main difference is that we are not providing a target variable like we did in supervised learning.

This marks a fundamental difference in how both types of algorithms operate. On one hand, we have supervised algorithms which try to minimize the error in classifying observations, while unsupervised learning algorithms don't have such gain, because there are no outcomes or target labels. Unsupervised algorithms try to create clusters of data that are inherently similar. In some cases we don't necessarily know what makes them similar, but the algorithms are capable of finding relationships between data points and group them in possible significant ways. Differently from supervised algorithms, which aim at minimizing the classification error, unsupervised algorithms try to create groups or subsets of the data, in which points belonging to a cluster are as similar to each other as possible, by making the difference between the clusters as high as possible (Haykin 1998).

Another main difference is that in an unsupervised problem, the concept of *training set* does not apply in the same way as with supervised learners. Typically we have a data set that is used to find the relationships in the data that buckets them in different clusters. A common workflow approach for unsupervised learning analysis is shown in the diagram below (Figure 14).

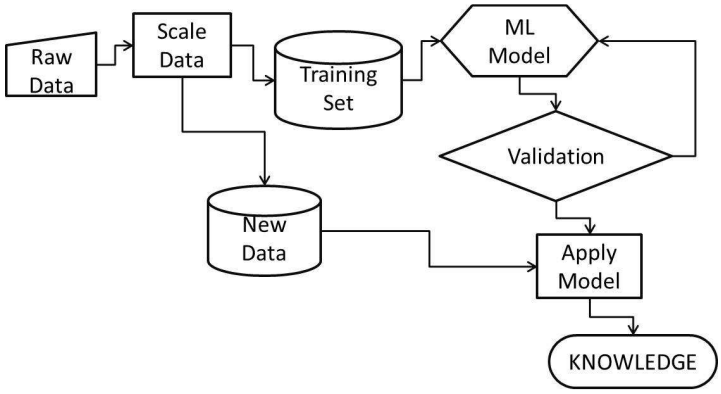


Figure 14 – A workflow based on unsupervised learning paradigm

For unsupervised learning, the process is:

1) *Pre-processing of data*. As with supervised learners, this step includes selection of features to feed into the algorithm, by also scaling them to build a suitable training data set;

2) *Execution of model training*. We run the unsupervised algorithm on the scaled data set to get groups of like observations;

3) *Validation.* After clustering the data, we need to verify whether it cleanly separated the data in significant ways. This includes calculating a set of statistics on the resulting outcomes, as well as analysis based on domain knowledge, where you may measure how certain features behave when aggregated by the clusters.

Once we are satisfied of the resulting creation of clusters (or in general over-densities), there is no need to run the model with new data (although you can).

4.2 What we are looking for in the data

In the DM scenario, the ML model choice should always be accompanied by the functionality domain. To be more precise, some ML models can be used in a same functionality domain, because it represents the functional context in which it is performed the exploration of data.

Traditional statistical methods break down partly because of the increase in the number of observations, but mostly because of the increase in the number of variables associated with each observation. The dimension of the data is the number of variables that are measured on each observation.

High-dimensional data sets present many mathematical challenges as well as some opportunities, and are bound to give rise to new theoretical developments. One of the problems with high-dimensional data sets is that, in many cases, not all the measured variables are "important" for understanding the underlying phenomena of interest. While certain computationally expensive novel methods can construct predictive models with high accuracy from high-dimensional data, it is still of interest in many applications to reduce the dimension of the original data prior to any data modeling (Samet 2006).

In mathematical terms, the problem we investigate can be stated as follows: given the p-dimensional random variable $x = (x^1, \cdots, x^p)^T$, and a lower dimensional representation of it, $s = (s^1, \cdots, s^k)^T$ with k ≤ p, that captures the content in the original data, according to some criterion. The components of s are sometimes called the hidden components. Different fields use different names for the p multivariate

vectors: the term “variable” is mostly used in statistics, while “feature” and “attribute” are alternatives commonly used in the DM and ML literature.

Generally speaking, dimensional reduction is the process of reducing the number of random variables under consideration, and can be divided into feature selection and feature extraction.

Feature selection approaches try to find a subset of the original variables (also called features or attributes) (Guyon et al. 2003). Two strategies are *filter* (e.g. information gain) and *wrapper* (e.g. search guided by the accuracy) approaches.

Feature extraction transforms the data in the high-dimensional space to a space of fewer dimensions. The data transformation may be linear, as in Principal Component Analysis (PCA), but many non-linear techniques also exist (Guyon et al. 2006).

Being based on the covariance matrix of the variables, PCA is a second-order method. In various fields, it is also known as the Singular Value Decomposition (SVD), the Karhunen-Loève transform, the Hotelling transform, and the Empirical Orthogonal Function (EOF) method. In essence, PCA seeks to reduce the dimension of the data by finding a few orthogonal linear combinations (Principal Components) of the original variables with the largest variance. In other words, PCA performs a linear mapping of the data to a lower dimensional space in such a way that the variance of the data in the low-dimensional representation is maximized.

Another technique belonging, like PCA, to the *latent variable* methods family, is the model known as Principal Probabilistic Surfaces (PPS), in which first principal component accounts for as much of the variability in the data as possible, and each

succeeding component accounts for as much of the remaining variability as possible (Chang et al. 2001).

The PPS are able to find a better data aggregation than the PCA method. A PPS is trained to recognize the best projection functions from the N-dimensional parameter space to a spherical surface in a 3D space.

This surface is covered by a grid of latent variables (points), representing the Gaussian peak in the N-parameter space. It permits to visualize all data with a human compliant 3D diagram, independently from the number of initial parameters. It is hence possible to individuate the presence of sub-structures in the data. An interesting aspect is the estimation of each input data parameter incidence on the latent variables that can help to understand the relationship between the parameter and the found clusters. The incidence of parameters is calculated by evaluating the probability density of input vector components in respect of each latent variable. During the training phase a reference variety is created.

In the test phase, a datum, never seen by the network, is attributed to the *closest* spherical variety. Obviously the concept of *closest* implies a calculation of a distance between a point and a node in the space. Before that the data must be projected on the space. This basically because a spherical variety consists of squared or triangular areas, each of them defined by 3 or 4 variety nodes. After this projection of the datum the approximated distance is calculated.

In the PPS system three main approximation criteria exist:

- Nearest Neighbor: it founds the minimum square distance from all variety nodes;
- Grid projections: it founds the shortest projection distance on the variety grid;

- Nearest Triangulation: it founds the projection closest to the possible triangulations.

The most frequently used is the first one, because it permits to evaluate the distances between data and all nodes on the spherical variety. The downside is that it is generally more time-consuming, but more precise than others (LeBlanc et al. 1994).

The technique described above makes clear the role of PPS as an efficient method for MDS pre-clustering or dimensional reduction.

More generally, the advantage to preliminarily apply a dimensional reduction model to data is that, in some cases, data analysis such as regression or classification can be done in the reduced space more accurately than in the original one.

Classification is a procedure in which individual items are placed into groups based on quantitative information on one or more features inherent to the items (referred to as features) and based on a training set of previously labeled items (Kotsiantis 2007).

A classifier is a system that performs a mapping from a feature space X to a set of labels Y. Basically a classifier assigns a pre-defined class label to a sample.

Formally, the problem can be stated as follows: given training data $\{(x_1, y_1), \cdots, (x_n, y_n)\}$ (where x_i are vectors) a classifier $h: X \rightarrow Y$ maps an object $x \in X$ to its classification label $y \in Y$.

Different classification problems could arise:

a) crispy classification: given an input pattern x (vector) the classifier returns its computed label y (scalar).

b) probabilistic classification: given an input pattern x (vector) the classifier returns a vector y which contains the probability of y_i to be the "right" label for x. In other words in this case we seek, for each input vector, the probability of its membership to the class y_i (for eachy_i).

Both cases may be applied to both "two-class" and "multi-class" classification. So the classification task involves, at least, three steps:

- training, by means of a training set (input: patterns and target vectors, or labels; output: an evaluation system of some sort);

- testing, by means of a test set (input: patterns and target vectors, requiring a valid evaluation system from point 1; output: some statistics about the test, confusion matrix, overall error, bit fail error, as well as the evaluated labels);

- evaluation, by means of an unlabeled data set (input: patterns, requiring a valid evaluation systems; output: the labels evaluated for each input pattern);

Because of the supervised nature of the classification task, the system performance can be measured by means of a test set during the testing procedure, in which unseen data are given to the system to be labeled.

The overall error somehow integrates information about the classification goodness. However, when a data set is unbalanced (when the number of samples in different classes varies greatly) the error rate of a classifier is not representative of the true performance of the classifier. A confusion matrix can be calculated to easily visualize the classification performance (Provost et al. 1998): each column of the matrix represents the instances in a predicted class, while each row represents the

instances in an actual class. One benefit of a confusion matrix is the simple way to see if the system is mixing two classes.

Optionally (some classification methods does not require it by its nature or simply as a user choice), one could need a validation procedure.

Validation is the process of checking if the classifier meets some criterion of generality when dealing with unseen data. It can be used to avoid over-fitting or to stop the training on the base of an "objective" criterion.

With “objective” we intend a criterion which is not based on the same data we have used for the training procedure. If the system does not meet this criterion it can be changed and then validated again, until the criterion is matched or a certain condition is reached (for example, the maximum number of epochs). There are different validation procedures. One can use an entire data set for validation purposes (thus called validation set); this data set can be prepared by the user directly or in an automatic fashion.

In some cases (e.g. when the training set is limited) one could want to apply a “cross validation” procedure, which means partitioning a sample of data into subsets such that the analysis is initially performed on a single subset, while the other subset(s) are retained for subsequent use in confirming and validating the initial analysis (Mosteller et al. 1968). Different types of cross validation may be implemented, e.g. k-fold, leave-one-out, etc.

Summarizing we can safely state that a common classification training task involves:

- the training set to compute the model;

- the validation set to choose the best parameters of this model (in case there are "additional" parameters that cannot be computed based on training);

- the test data as the final “judge”, to get an estimate of the quality on new data that are used neither to train the model, nor to determine its underlying parameters or structure or complexity of this model;

The validation set may be provided by the user, extracted from the software or generated dynamically in a cross validation procedure. In the next paragraphs we underline some practical aspects connected with the validation techniques for classification models.

Regression methods bring out relations between variables, especially whose relation is imperfect (i.e. it has not one y for each given x). The term regression is historically coming from biology in genetic transmission through generations, where for example it is known that tall fathers have tall sons, but not as tall on the average as the fathers. The trend to transmit on average genetic features, but not exactly in the same quantity, was what the scientist Galton defined as regression, more exactly *regression toward the mean* (Galton 1877).

But what is regression? Strictly speaking it is very difficult to find a precise definition. It seems the existence of two meanings for regression (Hastie et al. 2005), that can be addressed as data table statistical correlation (usually column averages) and as fitting of a function.

About the first meaning, let start with a very generic example: let’s suppose to have two variables x and y, where for each small interval of x there is a distribution of corresponding y. We can always compute a summary of the y values for that

interval. The summary might be for example the mean, median or even the geometric mean. Let fix the points $(x_i, \bar{y}_i)$, where x_i is the center of the ith interval and $\bar{y}_i$ the average y for that interval. Then the fixed points will fall close to a curve that could summarize them, possibly close to a straight line. Such a smooth curve approximates the regression curve called the regression of y on x. By generalizing the example, the typical application is when the user has a table (let say a series of input patterns coming from any experience or observation) with some correspondences between intervals of x (table rows) and some distributions of y (table columns), representing a generic correlation not well known (i.e. imperfect as introduced above) between them. Once we have such a table, we want for example to clarify or accent the relation between the specific values of one variable and the corresponding values of the other. If we want an average, we might compute the mean or median for each column. Then to get a regression, we might plot these averages against the midpoints of the class intervals.

Given the example in mind let's try to extrapolate the formal definition of regression (in its first meaning).

In a mathematical sense, when for each value of x there is a distribution of y, with density f(y|x) and the mean (or median) value of y for that x given by:

$$\bar{y}(x) = \int_{-\infty}^{+\infty} y f(y|x) dy \qquad (1)$$

then the function defined by the set of ordered pairs $(x, \bar{y}(x))$ is called the regression of y on x. Depending on the statistical operator used, the resulting regression line or curve on the same data can present a slightly different slope.

Sometimes we do not have continuous populations with known functional forms. But the data may be very extensive (such as in the astrophysical case). In these cases it is possible to break one of the variables into small intervals and compute averages for each of them. Then, without severe assumptions about the shape of the curve, essentially get a regression curve. What the regression curve does is essentially to give a, let say, "big summary" for the averages for the distributions corresponding to the set of x's. One can go further and compute several different regression curves corresponding to the various percentage points of the distributions and thus get a more complete picture of the input data set. Of course often it is an incomplete picture for a set of distributions! But in this first meaning of regression, when the data are more sparse, we may find that sampling variation makes impractical to get a reliable regression curve in the simple averaging way described (Menard 2001). From this assumption, it descends the second meaning of regression.

Usually it is possible to introduce a smoothing procedure, applying it either to the column summaries or to the original values of y's (of course after an ordering of y values in terms of increasing x). In other words we assume a shape for the curve describing the data, for example linear, quadratic, logarithmic or whatever. Then we fit the curve by some statistical method, often least-squares. In practice, we do not pretend that the resulting curve has the perfect shape of the regression curve that would arise if we had unlimited data, but simply we obtain an approximation. In other words we intend the regression of data in terms of forced fitting of a functional form. The real data present intrinsic conditions that make this second meaning as the official regression use case, instead of the first, i.e. curve connecting averages of

column distributions. We ordinarily choose for the curve a form with relatively few parameters and then we have to choose the method to fit it. In many manuals sometimes it might be founded a definition probably not formally perfect, but very clear: by regressing one y variable against one x variable means to find a carrier for x. This introduces possible more complicated scenarios in which more than one carrier of data can be founded. In these cases it has the advantage that the geometry can be kept to three dimensions (with two carriers) up to n-dimensional spaces (n > 3, with more than two carriers regressing input data). Clearly, both choosing the set of carriers from which a final subset is to be drawn and choosing that subset can be most disconcerting processes.

In substance we can declare a simple, important use of regression, consisting in:

To get a summary of data, i.e. to locate a representative functional operator of the data set, in a statistical sense (first meaning) or via an approximated trend curve estimation (second meaning).

And a more common use of regression:

- For evaluation of unknown features hidden into the data set;

- For prediction, as when we use information from several weather or astronomical seeing stations to predict the probability of rain or the turbulence growing in the atmosphere;

- For exclusion. Usually we may know that x affects y, and one could be curious to know whether z is associated with y too, through a possible casual mechanism. In this case one approach would take the effects of x out of y and see if what remains is associated with z. In practice this can be done by an iterative fitting procedure by evaluating at each step the residual of previous fitting.

This is not exhaustive of the regression argument, but simple considerations to help the understanding of the regression term and the possibility to extract basic specifications for the use case characterization in the design phase.

Clustering is a division of data into groups of similar objects. Representing the data by fewer clusters necessarily loses certain fine details (data compression), but achieves simplification (Jain et al. 1999).

From a ML perspective clusters correspond to hidden patterns, the search for clusters is unsupervised learning, and the resulting system could represent a data concept in the KDD (Knowledge Discovery in Databases).

From a practical perspective clustering plays an outstanding role in DM applications such as scientific data exploration, information retrieval and text mining, spatial database applications, Web analysis, Customer Relationships Management (CRM), marketing, medical diagnostics, computational biology, and many others.

For example, in CRM, marketing applications generally come with predictive clustering analytics to improve segmentation and targeting, and features for measuring the effectiveness of online, offline, and search marketing campaigns (Collica 2007). By evaluating “buy signals,” marketers can see which prospects are most likely to transact and also identify those who are bogged down in a sales process and need assistance.

Data mining on MDS adds to clustering the complications of very large data sets with very many attributes of different types (high dimensionality). This imposes unique computational requirements on relevant clustering algorithms.

What are the properties of clustering algorithms we are concerned with in DM?

These properties include:

- Type of attributes that the algorithm can handle;
- Scalability to large data sets;
- Ability to work with high dimensional data (multi-D parameter space, multi-wavelength, multi-epoch etc…);
- Ability to find clusters of irregular shape;
- Handling outliers;
- Time complexity (when there is no confusion, we use the term complexity);
- Data order dependency;
- Labeling or assignment (hard or strict vs. soft of fuzzy);
- Reliance on a priori knowledge and user defined parameters;
- Interpretability of results;

We have to try to keep these issues in mind, realistically. The above list is in no way exhaustive. For example, we must deal also with implementation properties, such as ability to work in pre-defined memory buffer, ability to restart and to provide an intermediate solution and so on.

4.3 Learning Strategies

Before going into the working mechanisms of ML systems, it is interesting and useful to focus the attention on the shape and expressions of data to be given as input to ML information processing models.

In ML experiments the performance strongly depends from data used for training. Hence it is crucial the choice of data selection and their representation mode.

Generally, except for some particular cases, the set of input data is provided under the form of tables or matrices; in which any row identify an example (a complete pattern in the data parameter space), whose columns are all parameters (features) and their values the parameter attributes.

It may be frequent that the table can have empty entries (sparse matrix) or missing (lack of observed values for some features in some patterns). It may also happen that information of a single table is not homogeneous, i. e. attributes may be of different types, such as numerical mixed with categorical entries.

This level of diversity in the internal information could be also related with different format type of data sets, such as tables registered in ASCII code (ANSI et al. 1977), CSV (Comma Separated Values) (Repici 2002) or FITS (text header followed by binary code of an image) (Wells et al. 1981).

In order to reach an efficient and homogeneous representation of data sets, to be submitted to ML systems, it is mandatory to preliminarily take care of the data format, in order to make them intelligible by the processing framework. In other words to transform pattern features to assume a uniform representation before to submit them to the training process.

In this mechanism the real situations could be very different. Let think to time sequences (coming from any sensor monitoring acquisition), where data are collected in a single long sequence, not simply divisible, or to raw data (such as

original images taken by astronomical observations), that could be affected by noise or aberration factors.

These events always require a pre-processing phase, to clean and opportunely prepare the data sets to be used for any ML and DM experiment. Of course such preliminary step must take into account also the functional scope of the experiment itself.

More in practice, having in mind the functional taxonomy described in the previous section, there are essentially four kinds of learning related with ML for DM:

1) Learning by association;
2) Learning by classification;
3) Learning by prediction;
4) Learning by grouping (clustering);

The primer, learning by association consists of the identification of any structure hidden between data. It does not mean to identify the belonging of patterns to specific classes, but to predict values of any feature attribute, by simply recalling it, i.e. by associating it to a particular state or sample of the real problem.

It is evident that in the case of association we are dealing with very generic problems, i.e. those requiring a precision less than in the classification case. In fact, the complexity grows with the range of possible multiple values for feature attributes, potentially causing a mismatch in the association results.

In practical terms, fixed percentage thresholds are given in order to reduce the mismatch occurrence for different association rules, based on the experience on that

problem and related data. The representation of data for associative learning is thus based on the labeling of features with non-numerical values or by alpha-numeric coding.

Classification learning is often named simply “supervised” learning, because the process to learn the right assignment of a label to a datum, representing its category or “class”, is usually done by examples. Learning by examples stands for a training scheme operating under supervision of any oracle, able to provide the correct, already known, outcome for each of the training sample. And this outcome is properly a class or category of the examples. Its representation depends on the available Base of Knowledge (BoK) and on its intrinsic nature, but in most cases is based on a series of numerical attributes, related to the extracted BoK, organized and submitted in a homogeneous way.

The success of classification learning is usually evaluated by trying out the acquired feature description on an independent set of data, having known output but never submitted to the model before.

Slightly different from classification scheme is the prediction learning. In this case the outcome consists of a numerical value instead of a class.

The numeric prediction is obviously related to a quantitative result, because is the predicted value much more interesting than the structure of the concept behind the numerical outcome.

Whenever there is no any class attribution, clustering learning is used to group data that show natural similar features. Of course the challenge of a clustering experiment is to find these clusters and assign input data to them. The data could be

given under the form of categorical/numerical tables and the success of a clustering process could be evaluated in terms of human experience on the problem or a posteriori by means of a second step of the experiment, in which a classification learning process is applied in order to learn an intelligent mechanism on how new data samples should be clustered.

In the wide variety of possible applications for ML, DM is of course one of the most important, but also the most challenging. Users encounter as much problems as massive is the data set to be investigated. To find hidden relationships between multiple features in thousands of patterns is hard, especially by considering the limited capacity of human brain to have a clear vision in a multiple than 3D parameter space.

Artificial neural networks are one of the best examples of ML methods, inspired by the human brain architecture and learning rules. Dealing with supervised learning, these models need training patterns formed by feature-target couples. Indeed for each given input pattern (list of features), there should be also given the corresponding list of targets (one or more). We already called such a complete data set as Base of Knowledge (BoK). With this data set, the network could be able to learn the right association between input features and location of its output in the parameter space. The network will be able, after this training process, to correctly classify any pattern, even if not presented to the network in the training phase (generalization).

One of the simplest models of supervised neural networks is the *Perceptron* (Rosenblatt 1957), composed by a single output neuron and N input neurons. The

capabilities of this model are very limited, but it is a good starting point for more advanced and complex variants of such network. The network learns by modifying the weights to enforce right decisions and discourage those wrong. At each iteration a new pattern of the training set is presented and the network calculates its output.

Main limit of such model is that it is able to correctly classify the input only if classes are linearly separable (see Figure 15a). However the division between classes is much more complex. A typical example is a problem (see Figure 15b), where it is not possible to find a single split line for the two classes and the Perceptron fails.

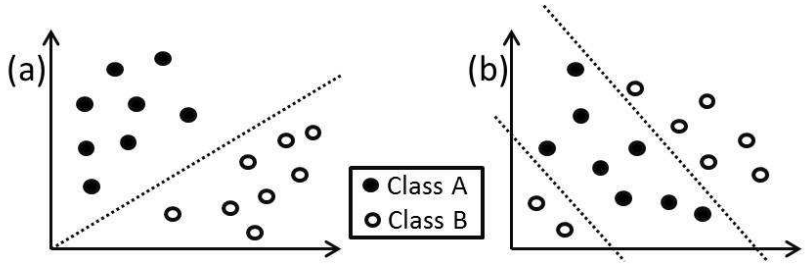


Figure 15 – correct (a) and wrong (b) separation of classes made by a Perceptron

To overcome this problem it is needed to employ more complex classification structures, organized on more than one computational layer (Cybenko 1989).

In order to be able to operate non-linear classification, i.e. to separate complex regions, the solution is to extend the perceptron to the so-called *Multi-Layer Perceptron* (MLP), a network composed by one or more hidden layers of neuron, fully connected, between input and output layers (Figure 16).

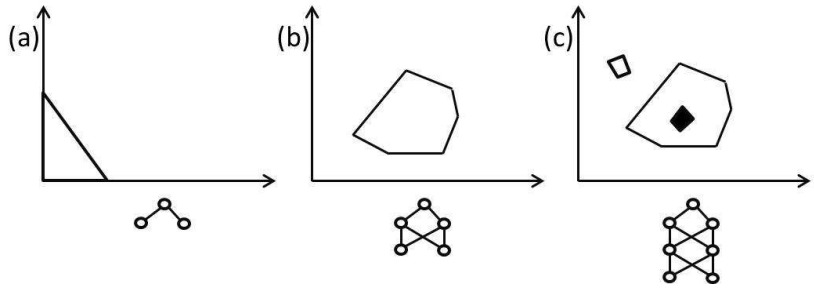


Figure 16 – Regions recognized by a MLP with 0, 1, 2 hidden layers

The classical topology of MLP is shown in Figure. This kind of networks is able to recognize and classify any type of topological region, having as downside a more complex learning process. Moreover, the Heaviside function cannot be applied as activation function, because it is not differentiable. An alternative is to use the sigmoid function. In this case the activation values of output neurons become differentiable functions of input values and hidden neuron weights.

The practice and expertise in the ML methods, such as MLP, are important factors, formed through a long exercise within scientific experiments. In particular the speed and effectiveness of the results strongly depend on these factors. Unfortunately there are no magic ways to a priori indicate the best configuration of internal parameters, involving network topology and learning algorithm, but a series of heuristics.

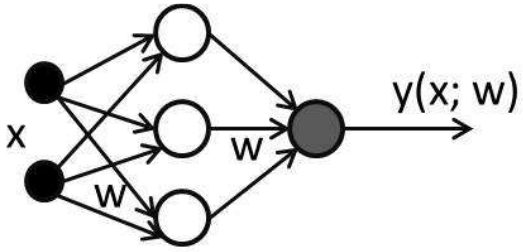


Figure 17 – Classical topology of a MLP with hidden neurons in white circles

Furthermore, if we define an error function as the Mean Square Error (MSE) between expected and network output, we found that it is a differentiable function of output and weights.

The learning process based on such rule is the so-called BackPropagation (BP), because the computed error is back propagated in the network from output to input layer (Rumelhart et al. 1986).

As shown, the BP learning rule tries to adapt weights in order to minimize the error function E(w). For networks without hidden layers, the error function will be squared and will assume a multi-dimensional parabolic shape, with only one absolute minimum. But for a generic MLP, the error function will be much more complex, with more than one minimum (local minima) in which the error gradient is zero Figure).

In these last cases it is important to distinguish between absolute and local minima. When, during the learning process, the error founds a local minimum, with the above adaption rule, the error function will not move anymore, resulting in a wrong (not absolute) minimization state.

There are basically two versions of the Descent Gradient Algorithm (hereinafter DGA): *online* and *batch*.

In the *online* version, referred to the above algorithm, the weights are updated after each input pattern presentation.

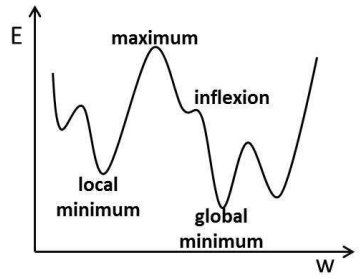


Figure 18 – typical behavior of error function during learning process

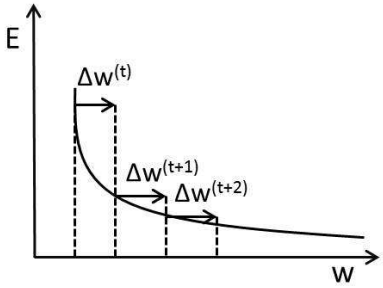


Figure 19 – The variation of weights on different error functions

In the *batch* version, the weights are updated after each presentation of the whole training set.

Between the two approaches, the first is preferable if there is a high degree of redundancy in the training set information, otherwise the second is the best.

Moreover, in all cases the descent gradient is not fast to converge. Fortunately there exist several methods to overcome these limits. In particular, in the batch case it results relatively easy to make DGA as a multi-threaded process, in which the training data sets are split into equally large batches for each of the threads (Heaton 2009).

Both versions require that the learning rate is a priori defined in a static way. This is another important point, because a high value of learning rate causes a more instable convergence of the learning process (the error function jumps along the error surface without convergence assurance). For a learning rate too small, the convergence will result extremely slowly.

The good compromise is to gradually reduce, at each learning step, the value of the learning rate (for example by simply following the law $\eta = 1/t$ or by applying more complex rules), obtaining a faster convergence of the algorithm (Jacobs 1988).

By using the standard DGA, the direction of each updating step is calculated through the error descent gradient, while the length is determined by the learning rate. A more sophisticated approach could be to move towards the negative direction of the gradient (*line search direction*) not by a fixed length, but up to reach the minimum of the function along that direction. This is possible by calculating the descent gradient and analyzing it with the variation of the learning rate.

The problem of *line search* is in practice a single dimension minimization problem. There exist many other methods to solve this problem. For example the parabolic search of a minimum calculates the parabolic curve crossing pre-defined learning rate points. The minimum d of the parabolic curve is a good approximation of the minimum of E(λ) and it can be reached by considering the parabolic curve crossing the fixed points with the lowest error values.

There are also the *trust region* based strategies to find a minimum of an error function, which main concept is to iteratively growing or contracting the region of the function by adjusting a quadratic model function which better approximates the

error function. In this sense this technique is considered dual to line search, because it tries to find the best size of the region by preliminarily fixing the moving step (the opposite of the line search strategy that always chooses the step direction before to select the step size), (Celis et al. 1985).

Up to now we have supposed that the optimal search direction for the method based on the *line search* is given at each step by the negative gradient. That's not always true!

If the minimization is done along the negative gradient, next search direction (the new gradient) will be orthogonal to the previous one. By selecting further directions equal to the negative gradient, there should be obtained some oscillations on the error function that slow down the convergence process. The solution could be to select further more directions such that the gradient component, parallel to the previous search direction (that is zero), remains unchanged at each step.

In the ML based on supervised paradigm, there is nowadays a considerable interest in techniques based on margin regularization (Baxter 2000). The concept derives from the assumption that the distance (typically Euclidean distance) of an example from the separating hyperplane is the margin of that example and the final goal is to find the best margin of separation (classification) for the submitted data. Significant examples include the Support Vector Machine (SVM), (Cortes et al. 1995), a powerful classification tool that has gained its popularity and interest due to its theoretical merits and successes in real applications (Burges 1998).

SVM were originally defined in order to classify two classes of objects linearly separable. For each class SVM identify the hyperplane that maximize the margin of separation (Figure 20).

In Figure 20 black dots are the first class, white dots the second class, the three lines are three possible margins, it is obvious that H3 is not suitable for this problem, H1 separates the two class but it's very near to some dots of the two class, H2 maximize the distance from the dots and is the best separator.

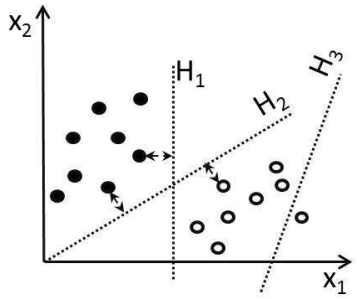


Figure 20 – Parameter space separated by hyperplanes through SVM model

Another technique related with the supervised ML is the one including methods called logic based algorithms. Main examples are *decision trees* or its derivation, rule-based estimators.

We have already introduced decision trees in the previous sections. By dealing with supervised learning, they try to classify patterns by sorting them on the base of their feature values.

However they have some defects. First, the construction of optimal binary decision trees is a well-known NP-complete problem (Hyafil et al. 1976), hence it requires complex heuristics to overcome this limit. Second, for their nature decision trees are

univariate, i.e. they split the parameter space on a single feature at each node, revealing inefficient in case of diagonal partitioning requirements. The solution is hence to use alternative multivariate trees, usually obtained by the combination between linear discriminant method and decision trees (Brodley et al. 1995).

As known, it is always possible to derive a rule-based estimator by a decision tree, simply associating one tree path to a separated rule.

One positive aspect of a decision tree is of course its comprehensibility and ease of use. It is intuitive enough to understand that a decision tree corresponds to a hierarchy of tests done by simply making the data flowing through the tree branches and taking output at its leaves (Kotsiantis 2007).

In the unsupervised case, the learning mechanism has something apparently magic. The data analysis model appears a closed system, except for the input data. It never interacts with external environment neither receives any kind of target outputs, but it learns!

Behind this apparently mysterious behavior, we can observe that the unsupervised learning consists in the internal re-organization of the input, based on the retrieved correlations hidden into the data by some quantities of unknown noise contributions. In a certain way, unsupervised learning can be interpreted as a self-adaptive mechanism to find patterns in the data beyond what can be considered pure unstructured noise (Gharamani 2004). Two important classic functional examples of such learning type are clustering and dimensional reduction.

Almost all unsupervised methods may be considered strictly connected with statistical and probabilistic issues. In this sense the final goal is to estimate a model

representing a probabilistic distribution of input data, conditioned by the previous sequence of data submitted to the system. Obviously the simplest case is when the ordering of the data sequence is irrelevant, because the variables are considered independent.

Under these conditions we can make use of the classical Bayesian rule (Berger 1985) in which, given a certain model A, considered as an unknown probability distribution over a data set S = {x1,…,xN}, the conditioned probability that the model fits the data is:

$$P(A|S) = \frac{P(A)P(S|A)}{P(S)} \quad (2)$$

And the corresponding model distribution, representing the estimation of the model output on new data can be expressed as:

$$P(x|S) = P(x|A)P(A|S) \quad (3)$$

An unsupervised model based on such considerations can be applied in many functional DM cases, such as classification, prediction, outlier detection and certainly data parameter space dimensional reduction.

Up to now we are making an important assumption, that is the input data are independent and distributed in an identical way. Although this is a very limiting condition, unreasonable in many real world cases, where current and incoming observed data are correlated with previous ones, it can be applied to time series analysis.

Many other clustering techniques are developed, primarily in ML, that either are used traditionally outside the DM community, or do not fit in previously outlined categories. They are basically specialized for KDD (Knowledge Discovery in Databases) and KDT (Knowledge Discovery in Text). There are relationships with unsupervised learning and evolutionary methods (simulated annealing and genetic algorithms). There is however the emerging field of constraint-based clustering (Tung et al. 2001), that is influenced by requirements of real world DM applications. Another frequently used technique in clustering is referred to the field of Artificial Neural Networks (ANN), in particular the model Self-Organized Map (SOM), (Kohonen 2007). SOM is very popular in many fields (such as vector quantization, image segmentation and clustering) and in this context its analytical description can be omitted, except for two important features: (i) SOM is based on the incremental approach, by processing one-by-one all input patterns; (ii) it allows to map centroids into 2D plane that provides for a quite simple visualization. In addition to SOM, other ANN developments, such as Adaptive Resonance Theory (ART), (Carpenter et al. 1991), or PPS have also relations with clustering.

4.4 The new generation of data mining infrastructures

As discussed in the previous chapter, the broad development and dissemination of Web 2.0 technologies have dramatically changed the perspective of how to make DM and analysis experiments, either from the user access and engineering design points of view. The huge dimensions of data, the recently discovered relevance of multi-disciplinary and cross correlation in modern DM and the advanced complexity

of ML methodologies have rapidly modified the requirements for applications and services to be made available to virtual communities of users, in industry, social networks, finance as well in all scientific and academic environments.

Such new requirements are indeed related with hardware computing infrastructures together with software tools, applications and services:

- Computing time efficiency, high storage systems, distributed multi-core processing farms and parallel programming: modern computing architectures, such as cloud, grid, HPC (High Performance Computing), GPU (Graphics Processing Unit) cannot be hosted by single user offices and require to concentrate computing facilities in data centers, accessible to worldwide user communities.

- The access to computing facilities must be as much as possible user-friendly, by embedding to the end user, potentially not technically skilled, all internal mechanisms and setup procedures;

- The remote access to data centers and analysis services must be asynchronous, in order to avoid the need for the user to maintain open the connection sockets for a potentially huge amount of time. It is in fact well known that massive data processing experiments, based on ML, are time-consuming;

- Data mining with ML methods are in principle structured as workflows (for example pipelines of data reduction and analysis in astrophysics), made by an ordered sequence of conceptual steps (data preparation, training, validation, test), one depending on each other. Any of the analysis and mining services must offer a complete set of tools to perform all these operational steps. In particular they should be able to offer scripting tools, to make custom setup and execution of different scripts, composed by various ML experiments automatically sequenced and ordered;

- Machine learning methods require a strong experience and both scientific and technological knowledge on their internal setup and learning mechanisms. In principle the end user should have an expert of ML techniques available during all phases of the experiments. So far, in the absence of human experts, the remote applications and services must guarantee the possibility to guide users through simple and intuitive interfaces to all conceptual steps of the experiments;

- Multi-disciplinary data centers must be interoperable, i.e. all archives require an high level of data format and access standardization in order to perform join and cross correlation activities in a fast and efficient way, without constraining a pre-treatment of data to obtain their uniformity and homogeneity;

- Massive data sets are often composed by GB or TB of data. It is unthinkable to make repetitive data moving operation on the network in a fast and efficient way. The use of metadata could represent a good compromise for any user who intends to manipulate data and to submit them to ML services in a remote way. So far, the available application frameworks must make available such mechanisms;

- The human machine as well as graphical user interfaces of remote data analysis systems should guarantee the interoperability between their ML engines, by making use of standards for algorithm description, setup and engineering. This could permit an efficient sharing mechanism between different data warehouses, avoiding replications of tools and confusion in the end users;

- In many scientific communities, users are accustomed to use their own algorithms and tools, sometimes specifically created to solve limited problems. Such tools were not originally designed by following programming standards or to be executed and portable on cross platforms. Modern ML service infrastructures should make available automatic plug-in features able to give to users the

possibility to integrate and execute their own scripts or algorithms on the remote computing platforms.

The above list of requirements is not exhaustive, but is sufficient to clear the important aspects related with what the modern virtual communities should expect to take full advantages of available Information and Communication Technologies (ICT) in the era of e-science.

Data mining with ML intrinsically contains so high levels of complexity and a wide degree of multi-disciplinary generalization to be a good candidate as benchmark for the new ICT solutions, being able to fully exploit its revolutionary features and products.

Currently there are a lot of applications and services, related to DM with ML, available in the world. Some of them were originally conceived for general purpose, others specialized to treat problems for a specific discipline or science/social community.

For example, DAMEWARE (Data Mining & Exploration Web Application REsource) is a rich internet application, one of the main products made available through the DAME international Program Collaboration. It provides a web browser based front-end, able to configure DM experiments on massive data sets and to execute them on a distributed computing infrastructure (cloud/grid hybrid platform), hidden to the users. DAMEWARE offers the possibility to access different DM functionalities (supervised classification, regression and clustering) implemented with different ML methods (among them, traditional MLPs, Support Vector Machines, Genetic Algorithms). Originally specialized and scientifically validated

on DM in Astrophysics, it can be used in a wide range of real problems and disciplines, by offering a completely transparent architecture, a user friendly interface, standards to ensure the long-term interoperability of data and the possibility to seamlessly access a distributed computing infrastructure. It also makes available an automatic tool to create user customable workflows and models, plugged in the application engine. In order to effectively deal with MDS, DAME offers asynchronous access to the infrastructure tools, thus allowing the running of activity jobs and processes outside the scope of any particular web application operation and without depending on the user connection status. The user, via a simple web browser, can access the application resources and can keep track of his jobs by recovering related information (partial/complete results) without having the need to maintain open the communication socket. Furthermore its GUI has widgets that make it interoperable with KNIME processing engine. The service is currently available as a beta release and under completion and test for some crucial aspects (experiment execution scheduling system, integration of new ML models, plug-in procedure). The main limit is the inability to setup and execute custom scripting procedures, constraining to manually setup and execute multiple ML experiments in a sequential way. The DAME Program website hosts other web-based services and resources for the astronomical virtual community, together with many documents useful especially for novices of ML techniques and DM methodology.

4.5 Selected strategy

Another important category of supervised ML models and techniques, in some way related with the Darwin's evolution law, is known as *evolutionary (*or *genetic) algorithms*, sometimes also defined as based on *genetic programming* (Michalewicz et al. 1996).

These names however present some differences. What we can surely assert is that Evolutionary or Genetic models are a category of algorithms that emulate the living organism evolution law. In the Nature all species follow that law in order to adapt their life style to the outdoor environment and to survive. In the ML paradigm this kind of self-adaptive methods try to solve optimization problems.

The relationship is strong between them, because the surviving can be considered an optimization problem as well.

The slight conceptual difference between evolutionary and genetic algorithms is that the formers are problem-dependent, while the latters are very generic. This is also a concept derived from the biologic models, in which all living species are commonly driven by genetic laws, but present specific internal mechanisms to achieve their proper evolution through population generations.

At the base of all evolutionary models there are some general concepts, present in both biological and ML models:

- Individuals as set of genetic features (chromosomes composed by genes);
- Population of individuals evolving in parallel;
- Reproduction of individuals based on re-combination operators and on random mutation;

- Selection of better individuals (solutions of the optimization problem) through fitness operators;

These common features are easily assembled in a form of computational algorithms and are demonstrated very effective by their success in the biological case. There could be also proved that such genetic programming rules are able to solve optimization (either minimization or maximization) problems, statistically converging to the best solution (Mitchell 1998).

In order to be more precise, the question is: what we intend for optimization problem solvable by genetic/evolutionary models?

Well, such problem must include some generic issues:

- Its solution depends on many parameters, to be evolved in strict combination between them;

- It must be always an optimization problem (minimization or its dual, maximization). This is easy to understand by thinking at the final goal of evolution in Nature, i.e. optimization of species adaptation;

- The optimization evaluation function (fitness function in evolutionary jargon) is a complex one, i.e. frequently it has not a closed mathematical expression. For instance, sometimes it is given under the form of a simulation of a real physical system;

- The problem has in principle unknown structure and complexity;

- The problem presents aspects or possible representations that could require a parallel processing. Genetic algorithms are intrinsically parallel, at different

levels, from lowest, in which the population members can be created and/or grown independently, to highest, where several independent populations can be grown in parallel or genetic operators can be applied to various population members in an independent way.

In all cases, genetic programming and evolutionary algorithms try always to mimic the evolution in Nature. With such issue in mind, it is easy to deduce that the genetic population corresponds to a set of possible optimization solutions to the given real problem.

The experience on such systems reveals that genetic and evolutionary algorithms are very generic, but if a specific algorithm could be created, it is very likely to be effective in the problem solving.

4.5.1 Data Quality Enhancement with data mining

In the traditional DQ methodology, briefly touched in the previous chapter, the statistical approach is usually employed for measuring the quality of data, in many common cases with good results (for example financial, enterprise, medical warehouses). But dealing with much more complex cases, especially in data warehouses designated as repositories of high precision scientific experiment results (like in the Euclid case), the traditional approach appears to be quite insufficient.

The major limit of statistical methods, when applied directly on data quality control, is the fact that traditionally DQ modifies the data themselves (Farzi et al. 2010) while for scientific data this needs to be avoided. Data Mining, on the contrary, is a methodology for measuring the quality of data, preserving their intrinsic nature. DM algorithms extract some knowledge that can be used to measure the quality of data,

with particular reference to the quality of input transactions and then, eventually flag the data of poor quality.

A typical procedure to measure DQ of data transactions should be based on three steps:

1. Extract all association rules, which depend on input transactions;
2. Select compatible association rules;
3. Add confidence factor of compatible rules as criteria of data quality of transaction.

There are two important challenging issues. First, the extraction of all association rules needs a lot of time and next, in most cases there is no exact mathematical formula for measuring data quality.

So far, a more effective DM approach to DQ should be alternative to find exact deterministic or statistical formulas. Therefore, for us, the answer is in employing methodologies derived from Machine Learning (ML) paradigms, such as (a) *active on-line learning*, which addresses the issue of optimizing the combination and trade-off of losses incurred during data acquisition; (b) *associative reinforcement learning*, (Kaelbling 1994), connected with the predictive quality of the final hypothesis.

Moreover, one of the guidelines of our proposed approach is to conjugate these machine learning paradigms with features coming from biological adaptive systems. The key principles are to process information systems using a connectionist approach to computation, in order to emulate the powerful correlation ability at the base of the cognitive learning engine of human brain (Gould 2002), together with the optimization process at the base of biological evolution (Darwin's law).

Our experience in such methodology has produced the DAME[14] (Data Mining & Exploration) Program, which includes several projects, mostly connected with Astrophysics, although spread into various of its scientific branches and sub-domains. Data Mining is usually conceived as an application (deterministic/stochastic algorithm) to extract unknown information from noisy data, (Dunham 2002). This is basically true but in some way it is too much reductive with respect to the wide range covered by mining concept domains. More precisely, in DAME, data mining is intended as techniques of exploration on data, based on the combination between parameter space filtering, machine learning and soft computing techniques associated to a functional domain. In the data mining scenario, the machine learning model choice should always be accompanied by the functionality domain. To be more precise, some machine learning models can be used in a same functionality domain, because it represents the functional context in which it is performed the exploration of data.

It needs to be stressed that, for what raw images streamed by the experiment are concerned, data quality would be based on the global and local properties of the images themselves, as well as on some a –priori constraints. For instance, on parameters, such as the average background counts, the filling factor of objects (i.e. number of pixels above a given flux threshold) as a function of many internal and external parameters (such as lim mag, galactic latitude, etc.). This implies the need

[14] http://dame.dsf.unina.it/

for an intelligent, reliable and fast on the fly segmentation of the image such as, for instance, that provided by the NExt-II software[15].

From the technological point of view, the employment of state of the art web 2.0 technologies, allows the end user (i.e. the data centers) to be in the best condition to interact with the DQ process by making use of a simple web browser.

The approach outlined above has three immediate advantages:

- DQ controls can be approached by remote, through homogeneous and interoperable interfaces, federated whereas possible under VO standards.

- Different DQ models and algorithms available by remote web applications can be tested by the end user (SDC) in a standard and intuitive way. In other words, the SDC does not need to be particularly skilled with DM methodologies to create and configure workflows on data;
- DM applications could be executed by remote cloud/grid frameworks, embedding all the complex management issues of the distributed computing infrastructure.

However, another indirect positive issue for our approach arises by considering that, in a massive data centric project like EDW, one of the unavoidable constraints is to minimize data flow traffic and down/up-load operations from remote sites. DQ tools should therefore be installed and maintained at the SDC.

It is worth to stress that this approach fits perfectly within the recently emerging area of interest named DQM (Data Quality Mining). DQ uses information attributes as a tool for assessing quality of data products. The goal of DQM is to employ data mining methods in order to detect, quantify, explain and correct DQ deficiencies in

[15] http://dame.dsf.unina.it/next.html

very large databases. For this reason there is a reciprocal advantage between the two application fields (DQ is crucial for many applications of KDD, which on the other side can improve DQ results).

4.5.2 Data Quality Mining and scalability issues

DQ and DQM are computing intensive and their computational cost grows quickly with the size and complexity of the data to be analyzed. In what follows we shortly describe how Graphic Processing Units (GPUs) could offer an effective and inexpensive way to deal with such problem even in the framework of a mission as complex as Euclid is.

In Euclid SGS warehouse the scientific quality control is particularly referred with data and metadata related to both images and spectra. Most of the KDD techniques based on machine learning that could directly be employed on such kind of data can be considered naturally parallel in terms of their analysis computation.

As an example let us consider a Multi Objective Genetic Algorithm (MOGA), based on the linkage between feature selections and association rules, that is one of the key concepts in the DQ methodology. The main motivation for using GA in the discovery of high-level prediction rules is that they perform a global search and cope better with attribute interaction, often used in DM problems (Das et al. 2009). Therefore a parallel GA further promotes the performance of computing, particularly required on massive data warehouse quality control.

A traditional parallel computing environment is very difficult and expensive to set up. This can be circumvented by recurring to graphics hardware, inexpensive, more

powerful, and perfectly comparable with other more complex HPC mainframes in terms of computing power (many frameworks based on GPU architecture are already included in the top 500 HPC worldwide supercomputer ranking[16]).

The DAME Program has already started the investigation on the design and implementation of a hierarchical parallel genetic algorithm, implemented on new technology based on multi-core Graphics Processing Unit (GPU) provided by NVIDIA Company, by using the Compute Unified Device Architecture (CUDA) parallel programming SDK. CUDA is a platform for massively parallel high-performance computing on the company's powerful GPUs (Zhang et al. 2009). At its cores are three key abstractions: (a) a hierarchy of thread groups, (b) shared memories, and (c) barrier synchronization that are simply exposed to the programmer as a minimal set of language extensions. These abstractions provide fine-grained data parallelism and thread parallelism, nested within coarse grained data parallelism and task parallelism.

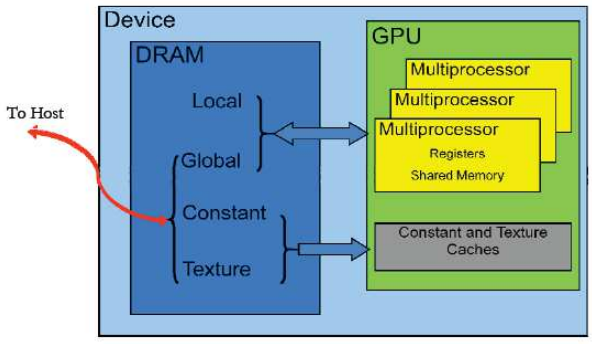


Figure 21 – GPU CUDA memory handling architecture

[16] http://www.top500.org/

The amount of performance benefit an application will realize by running on CUDA depends entirely on the extent to which it can be parallelized. As mentioned previously, code that cannot be sufficiently parallelized should run on the host, unless doing so would result in excessive transfers between host and device.

Amdahl's law specifies the maximum speed-up that can be expected by parallelizing portions of a serial program (Amdahl 1967). Essentially, it states that the maximum speed-up (*S*) of a program is:

$$S = \frac{1}{(1-P)+(P/N)} \quad (4)$$

where *P* is the fraction of the total serial execution time taken by the portion of code that can be parallelized and *N* is the number of processors over which the parallel portion of the code runs.

The larger *N* is (that is, the greater the number of processors), the smaller the *P/N* fraction. It can be simpler to view *N* as a very large number, which essentially transforms the equation into $S = 1/(1-P)$. For example, if ¾ of a program is parallelized, the maximum speed-up over serial code is $S = 1/\left(1-\frac{3}{4}\right) = 4$.

Moreover, effective bandwidth is calculated by timing specific program activities and by knowing his equation how data is accessed by the program. To do so, we can use the formula:

$$effective_{bandwidth} = \left({(B_r + B_w)}/{10^9} \right)/time \quad (5)$$

where the effective bandwidth is in units of GBps (Giga Byte per second), B_r is the number of bytes read per kernel, B_w is the number of bytes written per kernel, and time is given in seconds.

For example, to compute the effective bandwidth of a 2048 x 2048 matrix copy, the formula (5) could be used obtaining:

$$effective_{bandwidth} = \left({(2048^2 \times 4 \times 2)}/{10^9} \right) / time \qquad (6)$$

The number of elements is multiplied by the size of each element (4 bytes for a float), multiplied by 2 (because of the read *and* write), divided by 10^9 to obtain GB of memory transferred. This number is divided by the time in seconds to obtain GBps.

In our *vision* such mix between software DM and ML techniques together with hardware high performance at low cost distributed computation architecture, could engage and maintain an adequate level of reliability and performance in the DQ control during both the design and development stages of the Euclid Data Warehouse.

5 Genetic Algorithms within CUDA parallel architecture

Genetic Algorithms (GA) are methods inspired to natural evolution as described by Darwin. They are powerful instruments to solve problems where parameter space is not well defined to find best solution. They always ensure the convergence towards the best solution, avoiding typical limits of other algorithms, such as local minima.

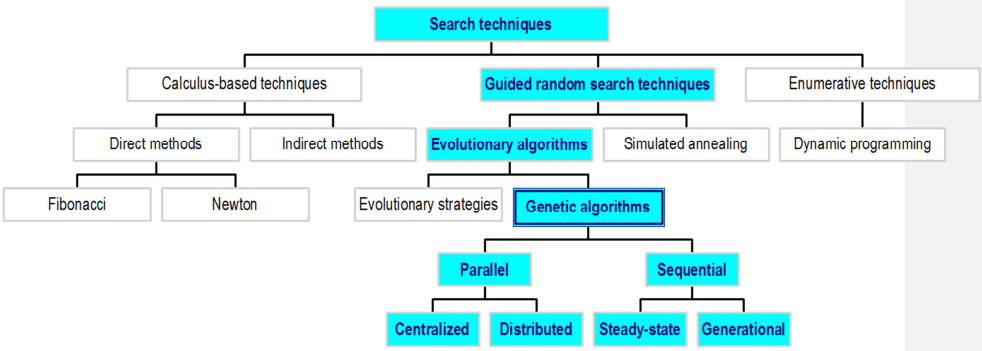


Figure 22 – Genetic Algorithms in the hierarchical search method taxonomy

GAME (Genetic Algorithm Mining Experiment) is a pure genetic algorithm specially designed to solve supervised optimizations problems related with regression or classification functionalities, scalable to efficiently manage Massive Data Sets (MDS) and based on the usual genetic evolution methods (crossover, genetic mutation, roulette/tournament, elitism).

GAME as a genetic algorithm needs the creation of chromosomes' population (genome), this means that we need an internal representation (encoding genes of the chromosomes, normalization) and a fitness function able to evaluate the goodness of a chromosome than other. This depends obviously from the problem examined and hence from nature and the intrinsic characteristics of the dataset evaluated.

In order to give a level of abstraction able to make simple adapt the algorithm to the specific problem, a family of polynomial developments was chosen. This methodology makes the algorithm itself easily expandable, but this abstraction requires a set of parameters that allows to fit the algorithm to the specific problem.

From an analytic point of view, a pattern, composed of N features contains an amount of information correlated between the features corresponding to the target value. Usually in a real scientific problem that correlation is "masked" from the noise (both intrinsic to the phenomenon, and due to the acquisition system); but the unknown correlation function can ever be approximated with a polynomial sequence; degree and non-linearity of the chosen function determine the approximation level, e.g. in the hybrid model GA+MLP, the polynomial sequence is represented from the weights of the net and from the activation function of neurons; hence the mathematical validity of the method is guaranteed and preserved.

The generic function of a polynomial sequence is based on these simple considerations:

Given a generic dataset with N features and a target *t*, *pat* a generic input pattern of the dataset, $pat = (f_1, \cdots, f_N, t)$ and *g(x)* a generic real function, the representation

of a generic feature f_i of a generic pattern, with a polynomial sequence of degree *d* is:

$$G(f_i) \cong a_0 + a_1\, g(f_i) + \cdots + a_d\, g^d(f_i) \tag{7}$$

Hence, the k-th pattern (pat_k) with N features may be represented by:

$$Out(pat_k) \cong \sum_{i=1}^{N} G(f_i) \cong a_0 + \sum_{i=1}^{N} \sum_{j=1}^{d} a_j\, g^j(f_i) \tag{8}$$

Then target t_k, concerning to pattern pat_k, can be used to evaluate the approximation error of the input pattern to the expected value:

$$E_k = (t_k - Out(pat_k))^2 \tag{9}$$

If we generalize the expression (8) to an entire dataset, with NP patterns number (k = 1, …, NP), at the end of the "forward" phase (batch) of the GA, we have NP expressions (8) which represent the polynomial approximation of the dataset.
In order to evaluate the fitness of the patterns as extension of (9) Mean Square Error (MSE) or Root Mean Square Error (RMSE) may be used:

$$MSE = \frac{\sum_{k=1}^{NP} (t_k - Out(pat_k))^2}{NP} \tag{10}$$

$$RMSE = \sqrt{\frac{\sum_{k=1}^{NP} (t_k - Out(pat_k))^2}{NP}} \tag{11}$$

Then we define a GA with this characteristic:

- The expression (8) is the fitness function;
- The array (a_0, …, a_M) defines M genes of the generic chromosome (initially they are generated random and normalized between -1 and +1);
- All the chromosomes have the same size (constrain from a classic GA);
- The expression (9) gives the standard error to evaluate the fitness level of the chromosomes;
- The population (genome) is composed by a number of chromosomes imposed from the choice of the function *g(x)* of the polynomial sequence.

About the last item we can say that this number is determined by the following expression:

$$NUM_{CHROMOSOMES} = (d \cdot N) + 1 \quad (12)$$

where *N* is the number of features of the patterns and *B* is a multiplicative factor that depends from the *g(x)* function, in the simplest case is just 1, but can arise to 3 or 4 in more complex cases.

A derivation of the Holland's theory (Holland 1975), states that the best solutions may be found using a population of 20, up to 50, chromosomes. By using much more chromosomes it doesn't help the convergence of the GA, also dramatically increasing the computational time.

The parameter *B* also influence the dimension of each chromosome (number of genes):

$$NUM_{GENES} = (d \cdot B) + 1 \quad (13)$$

where *d* is the degree of the polynomial.

For example if we use the trigonometric polynomial sequence, given by the following expression,

$$p(x) = a_0 + \sum_{m=1}^{n} a_m \cos(m\,x) + \sum_{m=1}^{n} b_m \sin(m\,x) \quad (14)$$

and to have 2000 patterns, each one with 11 features, the expression for the single (*k-th*) pattern, using (8) with degree 3, will be:

$$Out(pat_k) \cong \sum_{i=1}^{11} G(f_i) \cong a_0 + \sum_{i=1}^{11}\sum_{j=1}^{3} a_j\, cos(j\, f_i) + \sum_{i=1}^{11}\sum_{j=1}^{3} b_j\, sin(j\, f_i) \quad (15)$$

for $k = 1,\ldots,2000$.

In the (15) we have two groups of coefficients (sin and cosine), *B* will be 2, so the number of chromosomes for each generation will be:

$$NUM_{CHROMOSOMES} = (2 \cdot 11) + 1 = 23$$

Each chromosome will be composed by a number of genes given from (13):

$$NUM_{GENES} = (2 \cdot 3) + 1 = 7$$

Hence the generic genome (population at a generic evolution stage), will be composed by 23 chromosomes, each one with 7 genes [*a0, a1, a2, a3, b1, b2, b3*], with each single gene (coefficient of the polynomial) in the range $[-1, +1]$ and initially random generated.

By evaluating the goodness of a solution through MSE or RMSE metrics, sometimes it may happen that a better solution in terms of MSE is a worse solution for the model, for example if we have a simple crispy classification problem with two patterns (class types 0 and 1).

As an example, if the solutions are, respectively, 0.49 for the class 0 and 0.51 for the class 1, the efficiency is 100% (i.e. each pattern is correctly classified), with a MSE = 0.24. But a solution of 0 for the class 0 and 0.49 for the class 1 (efficiency of 50%), gives back a MSE = 0.13 and consequently the model will prefer the second solution, although with a lower efficiency.

In order to circumvent this problem, we decide to implement in GAME the so-called *convergence tube.*

Despite its name, its formulation is quite simple: for a given radius R the error within R is placed equal to 0 so that the equation (9) becomes:

if $abs\ (t_k - Out(pat_k))^2 > R \rightarrow E_k = (t_k - Out(pat_k))^2$

if $abs\ (t_k - Out(pat_k))^2 \leq R \rightarrow E_k = 0$ (16)

With the previous example, using R = 0.5, in the first case we have a MSE = 0, while in the second case MSE = 0.13, recognizing the first solution better than the second one and indeed revealing much better a correct trend according the efficiency of the algorithm.

5.1 GPU Design Model

To better address the GPU-based design starting from the serial implementation of the application, we choose to use an ad hoc software development methodology, for instance APOD (Assess, Parallelize, Optimize, and Deploy)(NVIDIA Corp. 2011).

APOD design cycle aims at quickly identify the portions of code that could take more easily the advantages and benefits of GPU acceleration, and begin to exploit the speedups resulting in production as fast as possible. APOD is a cyclical process: initial speedups can be achieved, tested, and deployed quickly, at which point the cycle can start over to identify further optimization opportunities.

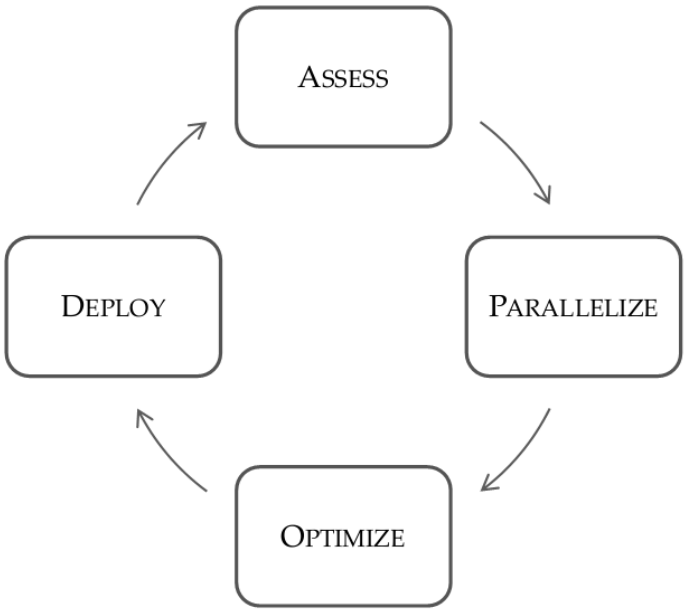


Figure 23 - APOD

5.1.1 Assess

The first step is to evaluate the multi-core application code to identify the parts responsible for most of the execution time. To identify the critical points and start to draw up a list of candidates for parallelization, the developers can use profiler tools. These bottlenecks are evaluated, de facto starting to investigate on parallelizable GPU acceleration. An upper limit of performance improvement can be estimated considering requirements and constraints, and by applying Amdahl's and Gustafson's laws (Gustafson 1988).

Gustafson's Law states that the problem size scales with the number of processors. Practically, for Gustafson the maximum speedup S of a program is:

$$S = N + (1 - P)(1 - N)$$

where P is the fraction of the total serial execution time taken by the portion of code that can be parallelized and N is the number of processors over which the parallel portion of the code runs.

5.1.2 Parallelize

Once identified the hotspots and having established the theoretical speedup achievable, we need to parallelize the code. By exposing the parallelism to improve performance and simply maintain the code of sequential applications, we are able to ensure also the maximum parallel throughput on GPU CUDA-capable. This could be as simple as adding a few preprocessor directives, such as OpenMP as

OpenACC, or it can be done by calling an existing GPU-optimized library such as cuBLAS, cuFFT, or Thrust.

Specifically, Thrust (Bell N. et al. 2010) is a parallel C++ template library like C++ STL (Standard Template Library) (Stepanov et al. 1995), it provides a rich collection of data parallel primitives such as *scan*, *sort*, and *reduce*, which can be composed together to implement complex algorithms with concise, readable source code. Thrust is implemented entirely within CUDA C/C++ and maintains interoperability with the rest of the CUDA ecosystem. The native interoperability with CUDA C is a powerful feature. Interoperability ensures that Thrust always complements CUDA C and that a Thrust plus CUDA C combination is never worse than either Thrust or CUDA C alone.

The Thrust library provides two vector containers: *host_vector* stored in host memory and *device_vector* lives in device memory and like the vector container in the C++ STL, both are generic containers that can be resized dynamically.

In Listing 2 acts on the vector containers using *generate*, *sort*, and *copy* algorithms. In this example, the iterators `h_vec.begin()` and `h_vec.end()` can be thought of as a pair of int pointers. Together the pair defines a range of integers of size `h_vec.end() - h_vec.begin()`.

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>
#include <thrust/sort.h>

int main(void)
{
   // generate 16M random numbers on the host
   thrust::host_vector<int> h_vec(1 << 24);
   thrust::generate(h_vec.begin(), h_vec.end(), rand);

   // transfer data to the device
   thrust::device_vector<int> d_vec = h_vec;

   // sort data on the device
   thrust::sort(d_vec.begin(), d_vec.end());

   // transfer data back to host
   thrust::copy(d_vec.begin(), d_vec.end(), h_vec.begin());

   return 0;
}
```

Listing 2 - Simple sort example using Thrust

Note that even though the computation implied by the call to the *sort* algorithm suggests one or more CUDA kernel launches, the programmer has not specified a launch configuration. Thrust's interface abstracts these details. The choice of performance-sensitive variables such as grid and block size, the details of memory management, and even the choice of sorting algorithm are left to the library implementations.

5.1.3 Optimize

After the parallelization step is complete, we can move to optimize the outcome to improve performance. As well APOD, optimization is an iterative process (identify an opportunity for optimization, apply and test optimization, verify the speedup achieved, and repeat), which means that it is not necessary to spend large amounts of time trying all possible optimization strategies. Instead, strategies can be applied

incrementally and using profiling tools can come in handy once again for guiding this process. Performance optimization is based on:

- Maximizing parallel execution;
- Optimizing memory usage to achieve maximum memory bandwidth;
- Optimizing instruction usage to achieve maximum instruction throughput.

Maximizing parallel execution starts with structuring the algorithm in order to expose as much "data parallelism" as possible. Once the parallelism of the algorithm has been exposed, should be mapped to the hardware as efficiently as possible. This is usually done by carefully choosing the running configuration of each kernel launch and maximizing competition between host and the device.

Optimizing memory usage starts by minimizing the host-to-device data transfers because they have much lower bandwidth than the device-to-device transfers. Sometimes, the best memory optimization could be simply to avoid any transfer of data by recalculating them whenever needed.

As for optimizing instruction usage, the use of arithmetic instructions that have low throughput should be avoided. This suggests trading precision for speed when it does not affect the end result, such as using single precision instead of double precision. Finally, particular attention must be paid to control flow instructions due to the SIMT (Single Instruction Multiple Thread) nature of the device.

5.1.4 Deploy

After completed an acceleration cycle, we can compare the result with the original implementation. Before tackling other critical points, the current partially

parallelized implementation is deployed. This allows us to profit from the improvements as fast as possible (the speed increase may be partial, but it is still valid).

With each generation of NVIDIA processors, new features are added to the GPU that CUDA can leverage. Consequently, it's important to understand the characteristics of the architecture. The computing capability describes the features of the hardware and reflects the set of instructions supported by the device as well as other specifications, such as the maximum number of threads per block and the number of registers per multiprocessor. Higher computing capability versions are backward compatible.

When in doubt about the computing capability of the hardware that will be present at runtime, it is best to assume a computing capability of 1.0 or 1.3, depending on the required double-precision arithmetic.

5.2 Multi-core Design Description

In a GA each element (called chromosome) has its DNA, in the form of a vector of genes, representing a potential solution to the problem.

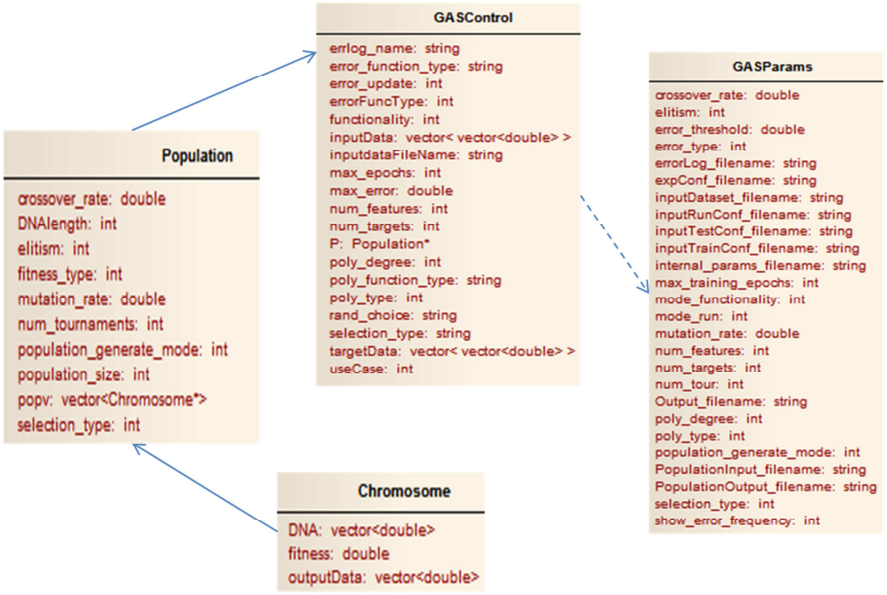


Figure 24 – GAME serial (multi-core) version class diagram

In particular, by referring to the class diagram of Figure 24, the crucial implementing aspects are:

the class **Chromosome** handles its own stack array `vector<double> DNA` with all genes and the stack array `vector<double> outputData`; which includes for each chromosome the vector of outputs for all input patterns. It must be taken into account that at the moment the program can execute experiments related to one-output (one-class or crispy) classification and one-output regression;

the class **Population** handles the stack array `vector<Chromosome*> popv`; that is a matrix with rows corresponding to the number of chromosomes and columns corresponding to the vector DNA of each chromosome;

the class **GASControl**, at an higher level, handles the object `Population *P`, and the stack matrices related to input and target patterns, respectively,

`vector<vector<double> > inputData`; and `vector<vector<double> > targetData`;

for the class **Population**, the most important methods are the constructor, `GASControl::GasControl`, which initializes the population and the method `GASControl::next`, which implements the population evolution during training;

Through several cycles, the population of chromosomes, originally created from a random generation (typically following the normal distribution), is replaced at each step by a new one obtained by applying genetic operators, trying to evolve it towards best population (solution). The DNA is usually a solution to a problem, codified (normalized) in order to permit an easier application of genetic operators. Typical representations used are the binary code or the values in [-1, 1] for each element (gene) of a chromosome. But sometimes, a normalization cannot be applied, depending on the problem topic area.

How a GA can evolve? Well, at the first stage, an initial random population is created.

There are available three types of random generation criteria:

- RANDOM: it generates pseudo-random values in [-1, +1];
- GRANDOM: it generates random values following the normal distribution in [-1, +1];
- DRANDOM: it generates pseudo-random values in [0, 1];

Then its chromosomes are evaluated in terms of their qualification to solve a specific problem, whose initial solutions are the chromosomes of the first random population. The evaluation is made by a specified **fitness function**. This operator

assigns a score to each chromosome. The best scored is the best solution for the current population. The choice of the best fitness function is one of the crucial design steps of a GA.

After the calculation of fitness operator for all chromosome of a generation, next step is the evolution (reproduction) of the population. The reproduction is done by using typical genetic operators, such as crossover, random mutation, whose common scope is to introduce genetic variety inside the original population, during the generation evolution. In practice, the reproduction is done by selecting stronger chromosomes and by killing others. But how to select them?

Obviously, the selection cannot be done randomly, otherwise the population will not evolve towards better solutions. The selection is done applying a well fixed fitness function.

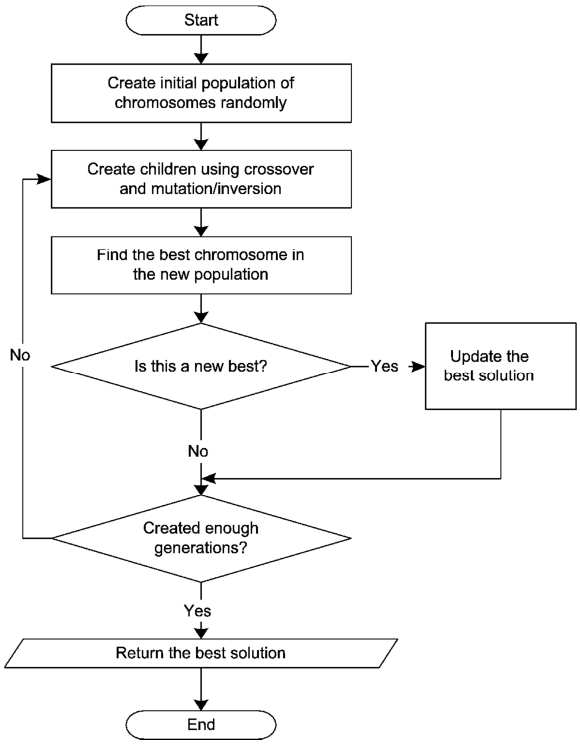


Figure 25 – Schematic block diagram for the execution flow of a GA

As mentioned above, the choice of the evaluation method to look for the best candidates to be reproduced over the generations of chromosomes, the so-called fitness function, is a crucial step in the GA design.

There is a large variety of possible fitness functions. One of the simplest is to codify chromosomes in an convenient way, such as BCD binary code, and then to compare a target value through its difference with the sum of half-groups of chromosomes.

In the present project, the idea is to use GA to solve supervised one-class classification and regression problems, typically related to an high-complexity parameter space where the background analytic function is not known, except for a

limited number of couples of input-target values, representing solutions to a physical category of phenomena.

In such cases, we want to train a GA to recognize the correct output to be assigned to other input samples extracted by real world cases. A typical case is to classify astronomical objects based on some solution samples (Base of Knowledge or BoK) and to learn to recognize new values extracted by further observations. To accomplish such behavior we designed a function (a polynomial expansion) to combine input patterns. The coefficients of these polynomials are the chromosome genes. The goal is to find the best chromosome so that the related polynomial expansion is able to approximate the right solutions to input pattern classification/regression.

So far, the fitness function for such representation consists of the error, obtained as absolute difference between the polynomial output and the target value for each pattern. Due to the fact that we are interested to find the minimum value of the error, the fitness is calculated as the opposite of the error (i.e. 1-error) and the problem is reduced to find the chromosome achieving the maximum value of fitness. At each evolution step (batch update of population) there are the following options, that can be chosen by user at configuration step:

- error function type: **MSE** (Mean Square Error), **TMSE** (Threshold MSE) or **RMSE** (Root MSE);

- selection type: the selection function to be used to extract some chromosomes as candidates to participate to the tournament, in order to be used to make evolution in the population. It is possible to choose between RANKING and ROULETTE type. In the **RANKING** case the winner chromosome is the one with the highest fitness. In

the **ROULETTE** the winner chromosome is selected with the highest probability, calculated as the ratio between its fitness and the sum of all chromosome fitness values inside the current population. It is called Roulette, because in the selection all chromosomes participate like in a classical roulette wheel random selection. In all the two cases above, the number of candidates chromosomes is randomly extracted from the current population (the number of candidates is one of the user selected parameters). After the tournament, the winner chromosome is used together with a new one, randomly created from scratch, to apply genetic operators (crossover and/or mutation).

- Another mechanism for evolving the population is the **Elitism**. It consists of a user selection of the number of copies of winner chromosome at current population, to be maintained as it is in the next generation, in order to preserve the best fitness obtained up to the current evolution step. This value should be taken low in order to don't waste members with worst fitness, that in any case, can play an important role during the entire evolution process. In fact we recall that the members with worst fitness play a not irrelevant role in the population evolution, because their "genetic material" can and must be subject of useful mesh inside the population during evolution, by applying genetic operators, such as crossover.

There are two genetic operators. They are used to mesh the genes between selected chromosomes (by one of the above tournament selection criteria).

Crossover happens when two chromosomes "break" themselves at the same point (inside the string coding the gene vector) and "exchange" their segments. For example, let's suppose to maintain the same fitness function of the example in the previous section:

(1) 00100101 (2 + 5 = 7) with fitness 15 - 7 = 8

(2) 00010111 (1 + 7 = 8) with fitness 15 - 8 = 7

Let's apply the crossover at index 3:

(1) 00100 101 → 00100 111 → 00100111 (2 + 7 = 9) with fitness 15 - 9 = 6

(2) 00010 111 → 00010 101 → 00010101 (1 + 5 = 6) with fitness 15 - 6 = 9

In the example, the chromosome son (1) has been optimized in terms of their fitness and it is a better solution than its fathers. The crossover implementation is at `Population::crossover`.

As all genetic operators, the crossover is not always applied in the genetic recombination, but with an associated probability (parameter `Population::crossover_rate`). While the breaking point inside the chromosome where to apply crossover is selected randomly (`int crosspoint = rand()length;`).

The **mutation** operator makes a single change in a gene of a chromosome, replacing it with a new value (`Population::Mutation`). As for crossover case, mutation is not always applied, but with a certain probability.

As mentioned above, the GA is implemented by a hierarchy of classes. The atomic element in this case is the class **Chromosome**, representing a single member of a population. It identifies a single vector of genes (coefficient of the polynomial expansion). A family of chromosomes is grouped in the class **Population**, representing a set of solutions (polynomial coefficients) racing in the selection of the best solution for the current problem identified by input patterns (user dataset).

The object of class **Chromosome** is identified by the vector of values in [-1, +1].

The constructor (`Chromosome::Chromosome`) creates a chromosome from scratch, assigning random values.

Inside this class there are various methods to manage genes. Main attributes are the vector DNA (the genes), fitness and the vector outputData (all output values for each input pattern related to the specific chromosome).

The class **Population** combines a set of chromosomes, plus a series of methods useful to perform crossover, reproduction etc...

The constructor is very simple. It takes as input the number of chromosomes of the population and set the population and chromosome sizes, by following formulas described above.

The method `Population::crossover` implements the genetic operator, already described above.

The method `Population::Mutation` implements the genetic operator, already described above.

The method `Population::getChromosomeFromRankTournament` implements the already mentioned RANKING selection criterion, providing the winner chromosome (candidate with best fitness, i.e. with lowest training error).

The method `Population::getChromosomeFromRouletteTournament` implements the already mentioned ROULETTE selection criterion, providing the winner chromosome (candidate with best fitness probability).

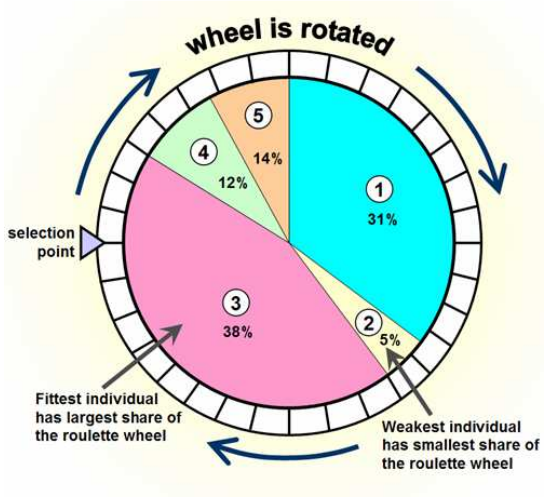


Figure 26 – Roulette selection technique

The methods `Population::best` and `Population::worst` are used to extract, respectively, winner and the worst candidate inside the current population, useful for the ordering of the chromosome vector.

Finally the overloading of the operator [ ] is a special mechanism useful to directly access to the members of population as being elements of a generic array, i.e. the same as for the specific method `Population::getMember`.

The reproduction, starting from the above array is done by the method `Population::next`, that applies genetic operators to obtain a new population. In this method it is important to mention the **elitism** mechanism. The elitism paradigm tries to maintain alive one or more copies of the best chromosome in the next population. This is done to prevent possible genetic modification of winner chromosome, causing its death during the evolution process, through several genetic recombinations of DNAs. The parameter (user defined) related to this elitism

mechanism defines the number of copies of the winner to be transmitted unchanged in the next population.

We recall also that the algorithm performs a **batch** error evaluation (i.e. by considering the error for each chromosome as calculated on the entire pattern set).

The project GAME is organized in functional portions, each one devoted to a specific use case to be executed.

The foreseen **use cases** are related to a typical machine learning model execution modes:

- TRAIN: the first mandatory case, consisting into submitting training datasets in order to build and store the best GA population, where best is in terms of its problem solving capability;

- TEST: case to be used in order to verify and validate the learning performance of the trained GA;

- RUN: the normal execution mode after training and validation;

- FULL: a workflow case, including in cascade TRAIN and TEST cases;

The choice of the current use case is done by user at setup time from external configuration files.

Also the **functionality** can be chosen by user. At the moment it is possible to run classification or regression types.

Depending on different use cases and experiments, the user should be able to perform a setup of many parameters and input/output files, without need to re-

compile the code. In order to implement this requirement, a set of input/output files has been designed.

5.2.1 Input Files

As input to the program (depending on specific use case) the user must provide following setup files:

- **input dataset** (input and/or desired output data)
- **specific experiment** (training/test/run) configuration file
- **specific use case** (train/test/full) configuration file

5.2.2 Input Dataset

The input dataset represents the input patterns to be processed for both training and/or test phases. These data must be submitted as an ASCII-file, with columns separated by spaces and without header. Each pattern must be filled in as a row vector. All patterns must be of the same size.

Depending on the specific use case, the input dataset should be made of:

The training and test dataset must consist of an ASCII file with first columns referred to input features, followed by (usually) two columns representing the targets (desired output) associated to each feature pattern.

EXAMPLE:

24.4753	-0.1139	1.822	51.29	0	1
22.6316	0.8065	5.002	80.45	1	0
22.4708	-0.3912	-7.425	5.66	0	1
23.9033	8.397	14.79	88.5	1	0

The above list is an example of an input dataset valid for training/test use cases, made of 4 patterns, with four feature columns, followed by two target columns.
In the other cases, run use case, only the feature columns must be present in the input file.

EXAMPLE:

24.4753	-0.1139	1.822	51.29
22.6316	0.8065	5.002	80.45
22.4708	-0.3912	-7.425	5.66
23.9033	8.397	14.79	88.5

This is the run use case version of the same train/test example, where the targets columns were removed.

5.2.3 Specific use case (training/test/run) configuration file

This group of files is related to the specific type of experiment the user wants to execute. There are three types of files: training, test and run setup.

In case of a **training** experiment, the user must provide an ASCII-coded file, with a specific format 38 rows x 1 column, whose meaning is the following:

- row 1 : <string> header label
- row 2 : <string> name of input dataset file
- row 3 : <string> header label
- row 4 : <string> initial population generation mode. It must be one of the following strings:
  RANDOM → pseudo-random generation in [-1, +1];
  DRANDOM → pseudo-random generation in [0, +1];
  GRANDOM → gaussian random generation in [-1, +1];
  NORANDOM → not random, but loaded from an external file (useful in case of training resume experiment);
- row 5 : <string> header label
- row 6 : <string> "none" or name of trained population file (depending on row 4)
- row 7 : <string> header label
- row 8 : <real> number of input features
- row 9 : <string> header label
- row 10: <integer> number of target columns
- row 11: <string> header label
- row 12: <real> order (max degree) of polynomial expansion
- row 13: <string> header label
- row 14: <string> type of polynomial expansion as combination for genes
  It can assume the following values:
  CL_POLY_TRIGO → trigonometric polynomial expansion (sum of sin and cosin);
- row 15: <string> header label
- row 16: <string> type of error calculation function. It can be:
  MSE → Mean Square Error
  TMSE → Thresholded Mean Square Error
  RMSE → Root Mean Square Error
- row 17: <string> header label

- row 18: <real> value of error rounded threshold (for TMSE only)
- row 19: <string> header label
- row 20: <string> type of selection function for evolving population. It can be:
  ROULETTE → uniform probability on entire population fitness function
  RANKING → absolute fitness rank of chromosomes
- row 21: <string> header label
- row 22: <real> error threshold (one of the stopping criteria)
- row 23: <string> header label
- row 24: <integer> max number of iterations (one of the stopping criteria)
- row 25: <string> header label
- row 26: <integer> frequency (number of iterations) of error reporting on stdout
- row 27: <string> header label
- row 28: <real> crossover (genetic operator) occurrence rate (range [0, 1])
- row 29: <string> header label
- row 30: <real> mutation (genetic operator) occurrence rate (range [0, 1])
- row 31: <string> header label
- row 32: <integer> number of chromosomes candidates to selection tournament
- row 33: <string> header label
- row 34: <integer> elitism factor (copies of winner into next generation)
- row 35: <string> header label
- row 36: <string> name of file where to store trained population
- row 37: <string> header label
- row 38: <string> name of output error log file
- row 39: <string> header label
- row 40: <string> name of GA output file

In case of **test/run** experiment, the user must provide an ASCII-coded file, with a specific format 8 rows x 1 column, whose meaning is the following:

- row 1 : <string> header label

- row 2 : <string> name of input test/run dataset file
- row 3 : <string> header label
- row 4 : <string> name of trained population file
- row 5 : <string> header label
- row 6 : <string> name of internal parameters file (fixed during training)
- row 7 : <string> header label
- row 8 : <string> name of test output file

5.2.4 Use case (train/test/run/full) configuration file

This group of files is related to the specific use case the user wants to launch. This is the main configuration file passed to the object Params through the constructor (class **GASParams**).

There are four types of files: train, test, run and full setup.

In case of **TRAIN**, **TEST** or **RUN** use cases, the ASCII-coded configuration file must contain the following information:

- row 1 : <string> header label
- row 2 : <string> functionality for the current experiment. It can be:
  CLASSIFICATION → classification (one-class) type
  REGRESSION → regression type
- row 3 : <string> header label
- row 4 : <string> name of use case. It can be:
  TRAIN → training use case type
  TEST → test use case type
  RUN → run use case
- row 5 : <string> header label
- row 6 : <string> name of input parameter setup file

In the **FULL** use case, the file has two more rows:

- row 1 : <string> header label
- row 2 : <string> functionality for the current experiment. It can be:
  CLASSIFICATION → classification (one-class) type
  REGRESSION → regression type
- row 3 : <string> header label
- row 4 : <string> name of use case. It must be:
  FULL → training+test use case type
- row 5 : <string> header label
- row 6 : <string> name of TRAIN input parameter setup file
- row 7 : <string> header label
- row 8 : <string> name of TEST input parameter setup file

5.2.5 Output Files

The output from the program strongly depends on specific use case).

Remember that for **FULL** use case, the outputs will be the sum of files obtained from training and test cases.

Common to all use cases (TRAIN, TEST, RUN) the output files are:

- GAME_<use case>_output.txt → the training data output file;
- GAME_<use case>.log → normal log status of the executed job;
- verbose_debug.log → a verbose log status report (the name is fixed);

Specific to **TRAIN** and **TEST** will be present also the following files;

- <functionality>_GAME_<use case>_confmat.txt → the confusion matrix for statistical results on the output;
- GAME_<use case>_error.txt → the list of errors at several cycles;
- internal_targets.txt → intermediate file (for internal use only);

Specific only to **TRAIN** will be present two more files;

- the trained population file;

- classification_trained_GAME_internal_params.txt → the list of used parameters as chosen by user. This file must be used for test/run cases;

5.3 Parallel Requirement Analysis

In all execution modes (use case), GAME exploits the `polyTrigo` function, consisting in a polynomial expansion in terms of sum of sines and cosines. Specifically in the Training use case, corresponding to the GA building and consolidation phase, the `polyTrigo()` is used at each iteration as the transformation function applied to each chromosome to obtain the output on the problem input dataset, and indirectly also to evaluate the fitness of each chromosome. It is indeed one of the critical aspects of the serial algorithm to be investigated during the parallelization design process.

Moreover, after having calculated the fitness function for all genetic population chromosomes, this information must be back-propagated to evaluate and evolving the genetic population (by using the selected genetic operators). This back and forth procedure must be replicated as many times as it is the training iteration number or the learning error threshold, both decided and imposed by the user at setup time of any experiment.

The direct consequence of the above issues is that the training use case takes much more execution time than the others and therefore is the one we are going to optimize. The key computational steps in this calculation loop are

1. generate initial population of chromosomes random.
2. calculate the fitness functions to find and order the best chromosomes in the population
3. evaluate the stop criteria (error or number of iteration)
4. stop or use the genetic evolution methods to evolve the population and goto 2

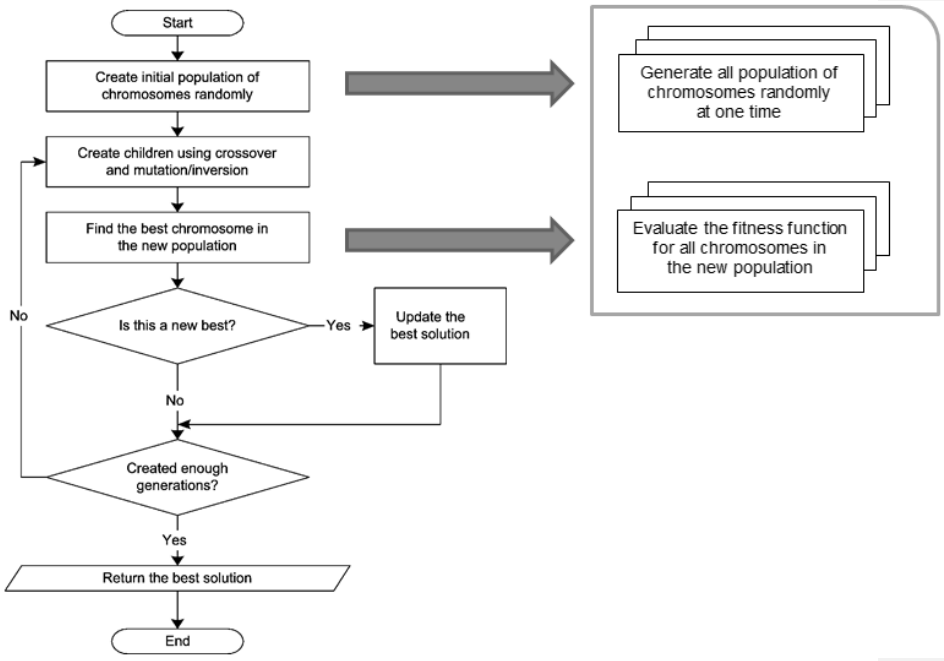


Figure 27- GA flow parallel specializations

Main design aspect approaching the software architecture analysis for the GPU is the partition of work: i.e. which work should be done on the CPU vs. the GPU.

As we can see in Figure 27, we have identified as time consuming critical parts, and hence potential tasks to be executed on the GPU, the generation of random population and the calculation of the fitness functions of chromosomes. For instance we focused the attention on these tasks as better candidates to exploit the data parallelism on the GPU.

In fact, the key principle is that we need to perform the same instruction simultaneously on as much data as possible. In random generation of population, the number of elements involved is never extremely large but it may

occur with an high frequency. This is because also during the population evolution loop a variable number of chromosomes are randomly generated to replace older individuals. To overcome this problem we may generate a large number of chromosomes randomly *una tantum*, by drawing elements from these whenever required. On the contrary, the evaluation of fitness functions involves all the input data, which is assumed to be massive datasets, so it already has an intrinsic data-parallelism.

5.4 GPU-based Development Description

5.4.1 Assess

Since CUDA programming involves code running concurrently on a host with one or more CPUs and one or more CUDA-enabled GPU devices where the devices have a dramatically different design from the hosts, it is important to keep in mind that these differences affect application performance to use CUDA effectively. To better exploit the resources, we have to use host and device together where the sequential work is done on the host and parallel work on the device. Which parts to run on the device? The device is designed for exploit massive data parallelism. This typically involves arithmetic operations on large datasets where the same operation can be performed on all dataset items.

To generate an application profile, we used Microsoft Visual Profiler which is the profiler that came with Microsoft Visual Studio 2010.

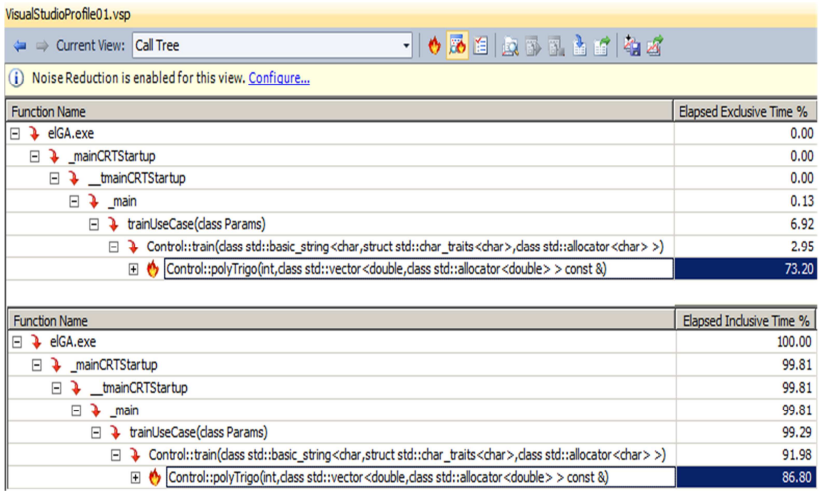


Figure 28 - Visual Profiler discover a Hotspot

In Figure 28, we can see that the function `polyTrigo()` (excluding its child functions) takes about three-quarters of the total execution time of the application while the total including child functions amounts to about 7/8 of total time execution. This will be our first candidate for parallelization.

It is worth noting that if other functions had taken a significant portion of total execution time, even if parallelizing these functions would increase our speedup, we would opted for parallelizing these functions in a later step because APOD is a cyclical process.

The benefits that can be achieved depend on the extent to which code can be parallelized. The code that cannot be well parallelized should be run on the host, unless that by doing so would lead to excessive host-to-device transfers.

Having analyzed the application profile, we apply either Amdahl's or Gustafson's Law to estimate an upper limit of the speedup achievable.

5.4.2 Parallelize

Once we have located a hotspot in our application's profile assessment and determined that custom code is the best approach, we can use Thrust library to expose the parallelism in that portion of our code as a call to an external function. We can then launch this external function onto the GPU and retrieve the results without requiring major rewrites to the rest of our application.

The function `polyTrigo()` was previously identified as candidate for parallelization and using Microsoft Visual Profiler we can check which of its statements is CPU time consuming.

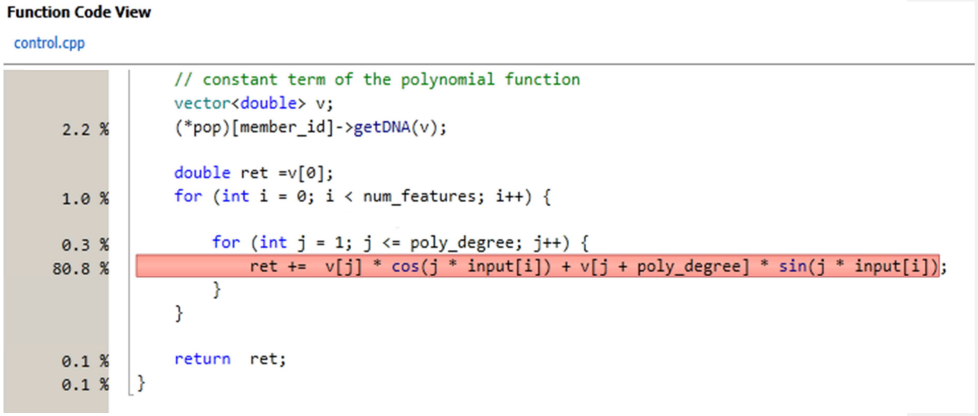


Figure 29 - `polyTrigo` instructions profile

Analyzing the instruction:

```
ret+=v[j]*cos(j*input[i])+v[j+poly_degree]*sin(j*input[i])
```

where `v[j]` is a vector containing DNA of a chromosome and `input[i]` is a vector containing a row of input dataset.

Noting that while the vector `v[]` is continually evolving, `input[]` (the elements of the input dataset) are being used in calculation of `ret` at each iteration but they are never altered, we rewrite the function by calculating in advance the sums of sines and cosines, storing the results in two vectors and then use them in the function `polyTrigo()` at each iteration.

This brings huge benefits because we calculate trigonometric functions, which are those time consuming, only once instead of at every iteration and exploit the parallelism on large amount of data because it assumes that we have large input datasets.

In Listing 3 we can see how the elements of vectors are calculated using Thrust

```
struct sinFunctor {

 __host__ __device__
 double operator()(thrust::tuple<double, double> t) {

  return sin(thrust::get < 0 > (t) * thrust::get < 1 > (t));
 }
};

struct cosFunctor {

 __host__ __device__
 double operator()(thrust::tuple<double,double > t) {

  return cos(thrust::get < 0 > (t) * thrust::get < 1 > (t));
 }
};

…

thrust::transform
 (thrust::make_zip_iterator
  (thrust::make_tuple(data.begin(),index.begin())),
 thrust::make_zip_iterator
  (thrust::make_tuple(data.end(),index.end())),
 tmpS.begin(),
 sinFunctor());
double s = reduce(tmpS.begin(),tmpS.end());
```

```
thrust::transform
 (thrust::make_zip_iterator
  (thrust::make_tuple(data.begin(),index.begin())),
 thrust::make_zip_iterator
  (thrust::make_tuple(data.end(),index.end())),
 tmpC.begin,
 cosFunctor());
double c = reduce(tmpC.begin(),tmpC.end());
…
```

Listing 3 – First parallelization

5.4.3 Optimize

Thrust's native CUDA C interoperability is a powerful feature. Interoperability ensures that Thrust always complements CUDA C and that a Thrust plus CUDA C combination is never worse than either Thrust or CUDA C alone. Indeed, while it may be possible to write whole parallel applications entirely with Thrust functions, it is often valuable to implement domain-specific functionality directly in CUDA C.

The level of abstraction targeted by native CUDA C affords programmers fine-grained control over the precise mapping of computational resources to a particular problem. Programming at this level provides developers the flexibility to implement specialized algorithms. Interoperability also facilitates an iterative optimization strategy: (1) quickly prototype a parallel application entirely in Thrust, (2) identify the application's hot spots, and (3) write more specialized algorithms in CUDA C and optimize as necessary.

So, to further improve the speedup it is possible to develop some algorithms in CUDA C by exploiting the interoperability, but we have skipped this step, by preferring a Thrust code optimization rather than a rewriting in CUDA. In brief, at the cost of lower speedup we gain rapid development and a better code readability.

There are three high-level optimization techniques that programmers may employ to yield significant performance speedups when using Thrust.

1. **Fusion**: In computations with low arithmetic intensity, the ratio of calculations per memory access, are constrained by the available memory bandwidth and do not fully exploits the GPU. One technique for increasing the computational intensity of an algorithm is to fuse multiple pipeline stages together into a single one.

```
for (int i = 0; i < N; i++)
   U[i] = F(X[i],Y[i],Z[i]);
                                  →
for (int i = 0; i < N; i++)
   V[i] = G(X[i],Y[i],Z[i]);
```

```
for (int i = 0; i < N; i++)
{
   U[i] = F(X[i],Y[i],Z[i]);
   V[i] = G(X[i],Y[i],Z[i]);
}
```

Listing 4 - Fusing Loops example

The simplest form of kernel fusion is *scalar function composition*.

```
for (int i = 0; i < N; i++)
   Y[i] = F(X[i]); (y=f(x))
                                  →
for (int i = 0; i < N; i++)
   sum += Y[i];   (z=g(y))
```

```
for (int i = 0; i < N; i++)
   sum += F(X[i]); (z=g(f(x)))
```

Listing 5 - Scalar Function Composition

In Thrust a better approach is to fuse the functions into a single operation $g(f(x))$ and halve the number of memory transactions. Unless f and g are computationally expensive operations, the fused implementation will run approximately twice as fast as the first approach.

Fusing a transformation with other algorithms is a worthwhile optimization. Thrust provides transform iterator which allows transformations to be fused with any algorithm. Indeed, `transform_reduce` is simply a convenience wrapper for the appropriate combination of `transform_iterator` and reduce.

2. **Structure of Arrays (SoA)**: An alternative way to improve memory efficiency is to ensure that all memory accesses benefit from coalescing, since coalesced memory access patterns are considerably faster than non-coalesced transactions.

   The most common violation of the memory coalescing rules arises when using an Array of Structures (AoS) data layout. An alternative to the AoS layout is the SoA approach, where the components of each struct are stored in separate arrays. The advantage of the SoA method is that regular access to its components of a given vector is coalesceable. The problem with SoA is that there is nothing to logically encapsulate the members of each element into a single entity.

   The `zip_iterator` takes a number of iterators and zip them together into a virtual range of tuples. Note that `zip_iterator` is used for both input and output ranges, transparently packing the underlying scalar ranges into tuples and then unpacking the tuples into the scalar ranges.

3. **Implicit Sequences**: the use of implicit ranges, i.e., ranges whose values are defined programmatically and not stored anywhere in memory. Thrust provides `counting_iterator`, which acts like an explicit range of values but does not carry any overhead. Specifically, when counting iterator is dereferenced it generates the appropriate value “on the fly” and yields that value to the caller.

```
typedef thrust::tuple<double, double> Tuple2;
// return the couple (cos(j*x), sin(j*x))
struct sincosFunctor {
  int deg;

  __host__ __device__
  tupleFunctor(int _deg) : deg(_deg) {
  }

  template <typename Tuple >
  __host__ __device__
  Tuple2 operator()(Tuple t) {
    int j= (thrust::get < 1 > (t) % deg) + 1;
    // Fusing Loops
    double c = cos(thrust::get < 0 > (t) * j);
    double s = sin(thrust::get < 0 > (t) * j);
    return Tuple2(c, s);
  }
};


…
Tuple2 result;
// fusion of transform with reduce algorithm
// (scalar function composition)
result = thrust::transform_reduce
  // SoA
 (thrust::make_zip_iterator
   (thrust::make_tuple
           // implicit sequence instead of stored vector
     (data.begin(),thrust::counting_iterator<int>(1))),
  thrust::make_zip_iterator
   (thrust::make_tuple
     (data.end(), thrust::counting_iterator<int>(myCol))),
  thrust::make_zip_iterator
   (thrust::make_tuple
     (tmpC.begin(), tmpS.begin())),
  sincosFunctor(poly_degree));
…
```

Listing 6 - Appling Transformations Optimizations

In Listing 6 has shown the optimized version of the code in Listing 3

5.4.4 Deploy

Results obtained using double-precision arithmetic will frequently differ from the same operation performed via single-precision arithmetic due to the greater precision of the former and due to rounding issues. Devices of compute capability 1.3 and higher provide native support for double-precision floating-point values. This means that whenever doubles are used, use at least the --arch=sm_13 option on the nvcc command line;

So, paying in terms of backward compatibility with old GPUs, we target to devices with computing capability of 1.3 and higher, given the importance of double precision in scientific computing.

6 Test results and performances

At this stage the CPU version of GAME, an optimized version of the serial algorithm (hereinafter Opt), where the parallelism is explained, and the final version for GPU (hereinafter ELGA) have been compared basically by measuring their performance in terms of execution speed. Initially, the tests have been organized by distinguishing between classification and regression functional modes. By analyzing early trials, however, it resulted that the performance growth was virtually achieved in both cases.

6.1 Metrics Definition

All data in the graphs refer to the average of five executions of the same experiment. It has served to mediate the various workloads about the CPUs and for the GPU to reduce the effect of an unexpected bias, a sort of transient from 4 to 6 seconds before the start of the first experiment run.

To measure the increase of performance, the speed, i.e. the ratio between the execution time of the serial version and the parallel one, has been calculated.

6.2 Comparison between Multi-core and GPU architectures

The performance of each use case was evaluated on several hardware platforms.

The input datasets were selected to be:

- representative for problems both in regression and classification;
- simulation data that researchers often work with;
- to exercise the limits of our algorithms, particularly in the case of the GPU.

We compared our production GPU code with a CPU implementation of the same algorithm. However, the CPU implementation's serial structure limited its computation to a single core.

The benchmarks were run on a 2.0 GHz Intel Core i7 2630QM quad core CPU running 64-bit Windows 7 Home Premium SP1. The CPU code was compiled using the Microsoft® C/C++ Optimizing Compiler version 16.00 and GPU benchmarks were performed using the NVIDIA CUDA programming toolkit version 4.1 running on several generations of NVIDIA GPUs GeForce GT540M.

6.3 Classification test

First of all we detail the results for a classification problem. Here we intend classification as defined in the case (a) described in section 4.2.

The input dataset chosen for classification is named GCSearch, a real dataset that refers to the following (Brescia et al. 2011b).

The scientific problem which is used here as a testbed for data mining applications is the study of GC populations in external galaxies. This topic is of interest to many astrophysical fields: from cosmology, to the evolution of stellar systems, to the formation and evolution of binary systems.

The study of Globular Clusters populations in external galaxies requires the use of wide-field, multi-band photometry. In fact GCs in galaxies more than a few Mpc

away, appear as unresolved sources in ground-based astronomical images and are thus hardly distinguishable from background galaxies, leading to severe contamination problems. For such reason they are traditionally selected based on source color and magnitude.

However, in order to minimize contamination and to measure GC properties, such as sizes and structural parameters (core radius, concentration, binary formation rates) high-resolution data are required as well, which are only available through the use of space facilities (i.e. Hubble Space Telescope, HST).

The dataset used in this experiment consists in wide field HST observations of the giant elliptical NGC1399 in the Fornax cluster. This galaxy represents an ideal test case since, due to its distance (20 Mpc), it is possible to cover a large fraction of its GC system with a limited number of observations. Furthermore at this distance GC are only marginally resolved even by HST, allowing to verify our experiment in a worst-case scenario. This dataset was used to study the GC-LMXB connection and the structural properties of the GC population.

The optical data were taken with the HST Advanced Camera for Surveys (ACS, program GO-10129), in the F606W filter, with integration time of 2108 seconds for each field. The observations were arranged in a 3x3 ACS mosaic, and combined into a single image using the MultiDrizzle routine. The final scale of the images is 0.03\arcsec/pix, providing Nyquist sampling of the ACS PSF. The field of view of the ACS mosaic covers ~100 square arcmin, extending out to a projected galactocentric distance of 55 kpc. The source catalog was generated with SExtractor, requiring a minimum area of 20 pixels. The NGC1399 region covered by our HST

mosaic, has no complete color coverage. In this experiment we will make use of two ancillary multi-wavelength datasets: archival HST g-z observations, which cover the very central region of the galaxy (10% of the sample), and ground based photometry. The latter is only available for 14% of our sources, and due to background light contamination, is very incomplete close to the galaxy center. In total 2740 sources of our catalog have multi-band photometry, Figure 30.

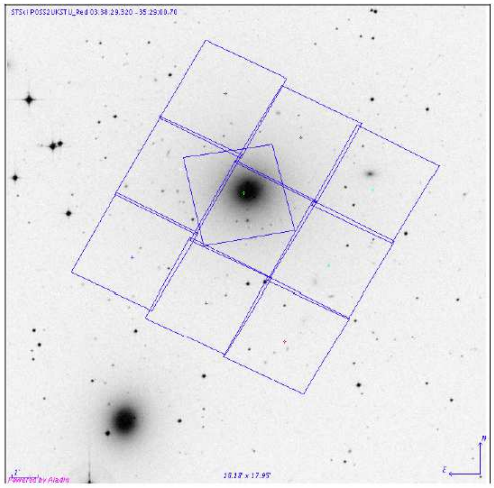


Figure 30 – The field of view (FOV) covered by the 3x3 HST/ACS mosaic in the F606W band. The central field, with a different orientation, shows the region covered by previous archival ACS observations in g and z bands.

The dataset file used consists of 2100 rows (input patterns) and 11 columns (features), 9 as input and last two as class targets (class labels, respectively, 0 for not GC and 1 for GC objects).

As execution parameters were chosen combinations of:

- max number of iterations: 1000, 2000, 4000, 10000, 20000 and 40000;

- order (max degree) of polynomial expansion: 1, 2, 4 and 8;

The other parameters remain unchanged for all test and they are setted as follow:

- Random mode for initial population: GRANDOM, generates random values following the normal distribution in [-1, +1].
- type of error function (fitness): Threshold Mean Square Error (TMSE).
- error threshold: 0.001 for Regression and 0.49 for Classification.
- selection type criterion: both RANKING and ROULETTE, types of selection function for evolving population.
- Error threshold: 0.001, used as a stopping criteria.
- Crossover rate: 0.9, occurrence rate of crossover genetic operator.
- Mutation rate: 0.2, occurrence rate of mutation genetic operator
- Number of tournament chromosomes: 4, number of chromosomes candidates to selection tournament.
- Elitism rate: 2, number of copies of winner chromosome into next generation.

6.3.1 Results

In this section we presented several graphs and tables which demonstrate the expected speed performance variation between the different computing architectures.

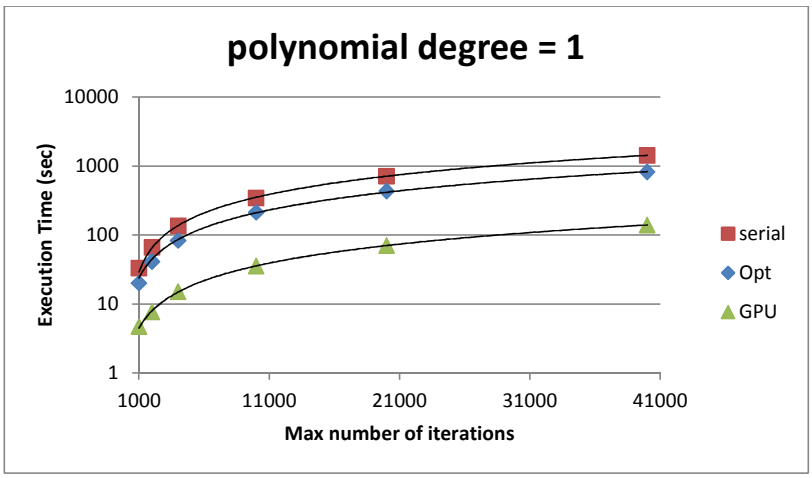


Figure 31 – Execution time comparison with degree=1

Commento [MB1]: Da aggiornare grafico

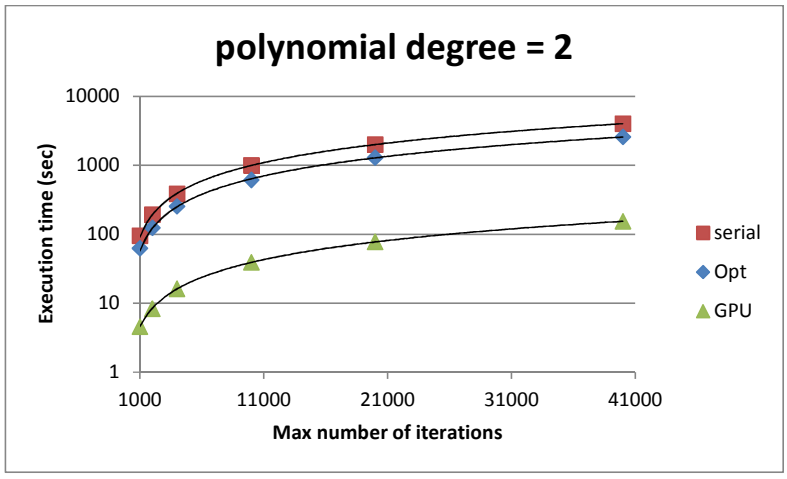


Figure 32 – Execution Time comparison with degree=2

Commento [MB2]: Da aggiornare grafico

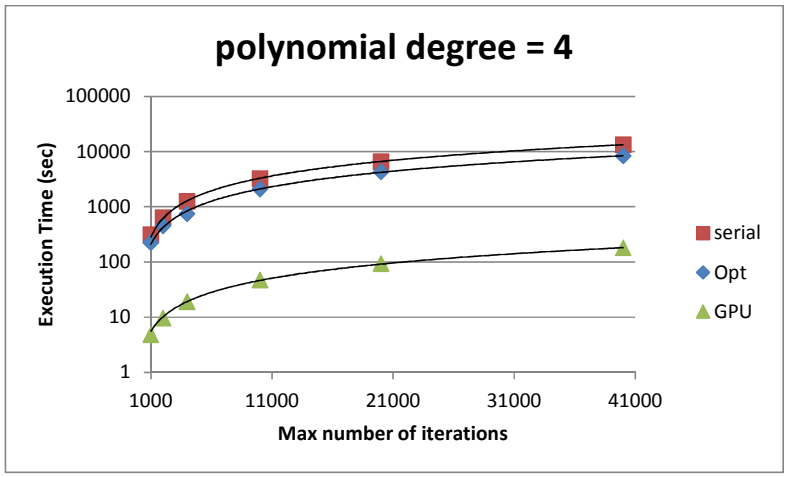


Figure 33 - Execution Time comparison with degree=4

Commento [MB3]: Da aggiornare grafico

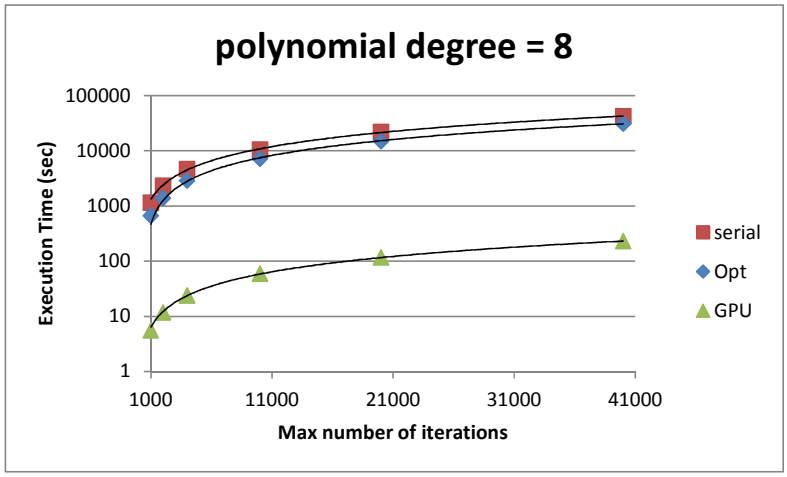


Figure 34 - Execution Time comparison with degree=8

Commento [MB4]: Da aggiornare grafico

The trends are immediately obvious from previous graphs. The execution time increases always in a linear way with the number of iterations fixed the polynomial

degree. This is what we expected since the algorithm repeats the same operations at each iteration.

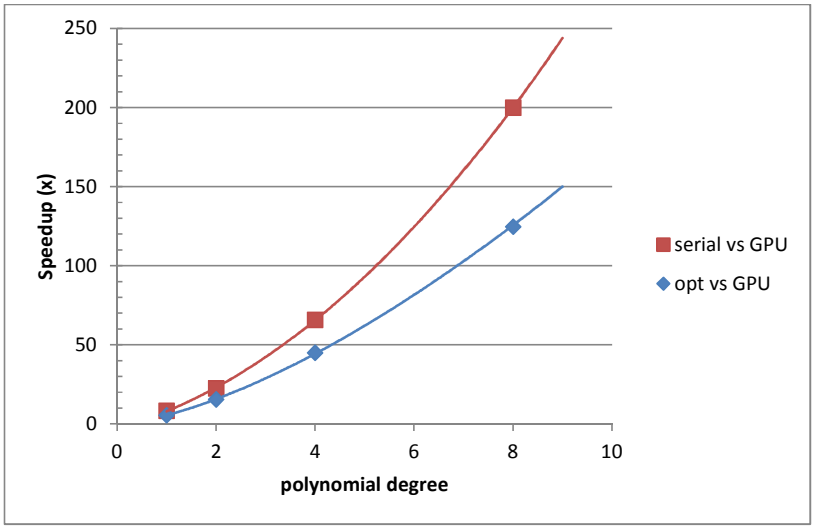


Figure 35 - Speedup comparison

In Figure 35, the speedup increases with a proportional factor of about 3 with increase of the maximum polynomial degree. This is because the GPU model requires a large number of genes, and so a greater degree, to be elaborate at the same time for effective speedup. This is typical for GPU algorithms, especially those relying on data parallelism.

Speedup				
degree	vs. Serial	step	vs. Opt	step
1	8x		6x	
2	23x	2.9	16x	2.7
4	66x	2.9	45x	2.8
8	200x	3.0	125x	2.8

Table 3 - Speed compared against CPU

The table lists results for the average speed in a range of iteration from 1000 to 40000 intended to show scaling performance for a very computationally demanding test case. Results come from comparison of parallel version against the initial version of the program (serial) and the optimized serial algorithm (Opt.).

The algorithm exploiting the data parallelism is as more powerful, as much data are simultaneously processed. As previously mentioned, an increase of maximum degree in the polynomial expansion leads to an increase in the number of genes and consequently to a larger population matrix. This may explain the upward trend in speedup shown in Table 3.

The GPU algorithm outperforms the CPU performance by a factor ranging from 8x to 200x in the first case and a range from 6x to 125x in the second one, enabling intensive use of the algorithm that were previously impossible to be achieved with a CPU.

6.4 Regression test

This section is dedicated to describe the results for a regression problem. Here we intend regression as defined in section 4.2.

The input dataset chosen for regression was constrained to be compliant with the sample selected for classification. Compliant means to maintain the same number of patterns (dataset rows) and features (dataset columns), in order to make both cases comparable in terms of speed performance evaluation.

In order to achieve this goal, we slightly modified the dataset used for classification, by adapting it to have same number of patterns and 11 columns, by assigning, respectively, first 10 columns as input features and the last one as the regression

target. The final scope of the problem was indeed to train the GA to learn the hidden correlation between the 10 features and the target one. Remember that all columns of original dataset were intrinsically correlated by the extraction of parameters from the reduced astronomical catalogue.

Of course, also the default GA parameters were maintained unchanged in respect of the classification test.

6.4.1 Results

As theoretically expected, by the choice of compliant datasets for classification and regression cases, the speed performances and comparisons show perfectly identical results and trends as already shown in the classification test report.

So far, we omit here to report the graphs and tables, because exactly the same of the previous ones, already shown in section 6.3.1.

Moreover, the perfectly analogous results for classification and regression functional cases demonstrate the consistency of the implementation for the three different computing architectures.

7 Conclusions and future developments

7.1 Conclusions

The original work of this thesis has touched on various topics. First of all, it was investigated the state of the art computing technologies, in order to choose the one best suited to our problem and later a multi-purpose genetic algorithm implemented with GPGPU / CUDA parallel computing technology has been designed and developed. The model comes from the machine paradigm of supervised learning, addressing both the problems of classification and regression applied on massive data sets. The model was derived from a serial implementation named GAME, deployed on the DAME Program hybrid distributed infrastructure and already scientifically tested and validated on astrophysics massive data sets problems with successful results (Brescia et al. 2011b).

Since genetic algorithms are inherently parallel, the parallel computing paradigm has provided an exploit of the internal training features of the model, permitting a strong optimization in terms of processing performances.

We described our effort to adapt our genetic algorithm for general purpose on GPU. We showed how this algorithm can be redesigned to efficiently use Thrust, the vendor-provided library routines. We discussed the efficiency and computational

costs of various components involved that are present in the algorithm. Several benchmark results were shown and the final test simulations were performed for Regression and Classification use.

The use of CUDA translates into a 75x average speedup. Clearly, we have been successful at eliminating the largest bottleneck in the CPU code. Although a speedup of up to 200X over a modern CPU is impressive, it ignores the larger picture of use a Genetic Algorithm as a whole. In any real-world the dataset can be very large (those we have previously called Massive Data Sets) and this requires greater attention to GPU memory management, in terms of scheduling and data transfers host-to-device and vice versa.

Moreover, the identical results for classification and regression functional cases, based also taking into account the constraints to maintain the structure of datasets perfectly compliant in both cases, demonstrate the consistency of the implementation for the three different computing architectures.

7.2 Future Work

We presented our experimental implementation of parallel Genetic Algorithm on GPUs. In our future development we are investigating possible optimizations.

The next step will be:

- Moving the formation of the population matrix and its evolution in place on the GPU, this approach has the potential to significantly reduce the number of operations in the core computation, but at the cost of higher memory usage.

- Exploring more improvement by mixing Thrust and CUDA C code, that should allow a modest speedup justifying development efforts at a lower level.

- Use of new features available on NVIDIA's Fermi architecture, such as faster atomics and more robust thread synchronization and multi GPUs capability.

After these optimizations, we plan to use this method in the ESA mission EUCLID for data quality.

A second direction for further work is the implementation of following Machine Learning algorithms, inspired by the models provided by DAME: Support Vector Machine (SVM), Multilayer Perceptron (MLP) and Probabilistic Principal Surfaces (PPS).

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9 References

Aha, W.; Kibler, D.; Albert, M.K., *Instance-Based Learning Algorithms*. 1991, Machine Learning, Kluwer Academic Publishers, Boston MA, USA, Vol. 6, pp.37-66.

Aho, A. V.; Hopcroft, J. E.; Ullman, J. D., *Data Structures and Algorithms.* Addison-Wesley, 1983. ISBN 0-201-00023-7.

Aldrich, J., R.A. *Fisher and the making of maximum likelihood* 1912–1922. 1997, Statistical Science 12 (3), pp. 162–176.

Amdahl, G.; *Validity of the Single Processor Approach to Achieving Large-Scale Computing Capabilities*. 1967, AFIPS Conference Proceedings (30): 483–485.

American National Standards Institute, et al. 1977, *American National Standard Code for Information Interchange.* The Institute.

Armstrong, J. S., *Principles of forecasting: a handbook for researchers and practitioners*, 2001, Kluwer Academic Publishers, Norwell, Massachusetts, ISBN 0-7923-7930-6.

Baum, E.; Wilczek, F., *Supervised learning of probability distributions by neural networks.* 1988, Neural Information Processing Systems, Anderson, D.Z. ed., American Institute of Physics, New York, pp. 52-61.

Baum, L.E.; Petrie, T., *Statistical inference for probabilistic functions of finite state Markov chains*, 1966. Annals of Mathematical Statistics, Vol. 37, Nr.6.

Bell, N.; Hoberock J., *Thrust: A Productivity-Oriented Library for CUDA.* 2011, *GPU Computing Gems, Jade Edition, Hwu* W., pp. 359-371, Morgan Kaufmann, ISBN: 0123859638.Berger, J. O., *Statistical decision theory and Bayesian Analysis*. 1985, 2nd ed., Springer-Verlag, New York.

Berkhin, P. 2002, *Survey Of Clustering Data Mining Techniques*, Technical Report, Accrue Software Inc.

Bijaoui, A.; Rué, F., *A Multiscale Vision Model*, 1995, Signal Processing Nr. 46, Vol. 345.

Bishop, C.M., *Pattern Recognition and Machine Learning*, 2006, Springer ISBN 0-387-31073-8.

Borne, K.D., *AstroInformatics: A 21st Century Approach to Astronomy*. 2009, in Astro2010 Decadal Survey State of the Profession, arXiv: 0909.3892v1.

Bray, T.; Paoli, J.; Sperberg-McQueen, C. M.; Maler, E.; Yergeau, F.; Cowan, J., XML 1.1 (Second Edition). 2006, W3C *Recommendation*, http://www.w3.org/TR/2006/REC-xml11-20060816/

Breiman, L.; Friedman, J.; Ohlsen, R.; Stone, C., *Classification and regression trees.* 1984, Wadsworth, Belmont, CA.

Brescia, M.; Longo, G.; Pasian, F., *Nuclear Instruments and Methods in Physics Research* 2010, Section A, Elsevier Science, Vol. 623, Issue 2, pp. 845-849, ISSN 0168-9002.

Brescia, M.; Longo, G., Euclid Consortium Scientific Ground Segment Data Quality Mining. 2011, Technical Communication to Euclid Consortium, document code EUCL-OAC-SGS-TN-00085.

Brescia, M.; Cavuoti, S.; Paolillo, M.; Longo, G.; Puzia, T.; The Detection of Globular Clusters in galaxies as a data mining problem. 2011b, accepted by MNRAS (in press), 11 pages, electronically available at arXiv: 1110.2144v1.

Brodley, C.E.; Utgoff, P.E., *Multivariate Decision trees*. 1995, Journal of Machine Learning, Kluwer Academic Publishers, Hingham, MA, USA, Vol. 19, Issue 1, pp. 45-77.

Broyden, C. G., *The convergence of a class of double-rank minimization algorithms.* 1970, Journal of the Institute of Mathematics and Its Applications, Vol. 6, pp. 76–90.

Burges, C.J.C., *A tutorial on support vector machines for pattern recognition.* 1998, Data Mining and Knowledge Discovery, Vol. 2, pp. 955-974.

Cabena, P.; Hadjinian, P.; Stadler, R.; Verhees, J. & Zanasi, A., *Discovering Data Mining: From Concepts to Implementation.* 1998, Prentice Hall.

Carpenter, G.A.; Grossberg, S.; Rosen, D.B, Fuzzy art: *Fast stable learning and categorization of analog patterns by an adaptive resonance system*. 1991, Neural Networks, Vol. 4, pp. 759-771.

Celis, M.; Dennis, J. E.; Tapia, R. A., *A trust region strategy for nonlinear equality constrained optimization.* 1985, in Numerical Optimization, P. Boggs, R. Byrd and R. Schnabel eds, SIAM, Philadelphia USA, pp. 71–82.

Chang, C. C., Lin, C. J., *Training Support Vector Classifiers: Theory and algorithms*, 2001. In Neural Computation, Vol. 13, pp. 2119-2147.

Chang, C. C., Lin, C. J., *LIBSVM: a library for support vector machines*. 2011, ACM Transactions on Intelligent Systems and Technology, Vol. 2, pp. 1-27.

Chang, K.; Ghosh, J., *Unified model for probabilistic principal surfaces*, IEEE Transactions on Pattern Analysis and Machine Intelligence, Publisher: IEEE, 2001, Vol. 23, pp. 22-41.

Clark, L. A; Pregibon, D., Tree-based models, 1992, In Statistical Models in Statistics, eds J. M. Chambers and T. J. Hastie, Chapter 9. New York, Chapman & Hall.

Collica R. S. 2007, *CRM Segmentation and Clustering Using SAS Enterprise* Miner, SAS Publishing, p. 290.

Cortes, C.; Vapnik, V., *Support-Vector Networks*. 1995, Machine Learning, Vol. 20.

Cybenko, G., *Approximation by superpositions of a sigmoidal function*. 1989, Mathematics of Control, Signals, and Systems, Vol. 2, pp. 303–314.

Das, S.; Saha, B.; Data Quality Mining using Genetic Algorithm. 2009, (IJCSS) Volume (3): Issue (2), 105-112.

Duda, R.O., Hart, P.E., Stork, D.G., 2001, *Pattern Classification*, A Wiley-Interscience Publication, New York USA, ISBN 0-471-05669-3.

Dunham, M.; *Data Mining Introductory and Advanced Topics*. 2002, Prentice-Hall.

Ebert, D.S.; Kenton Musgrave, F.; Peachey, D.; Perlin, K.; Worley, S.; *Texturing and modeling: a procedural approach*. 2000, AP Professional, ISBN 0-12-228730-4.

Fabbiano, G.; Calzetti, D.; Carilli, C.; Djorgovski, S. G.; *Recommendations of the VAO-Science Council*, 2010, arXiv:1006.2168v1 [astro-ph.IM].

Farzi, S.; Dastjerdi, A.; Data Quality Measurement using Data Mining. 2010, IJCTE Vol. 2, No. 1, 1793-8201.

Fletcher, R., *A New Approach to Variable Metric Algorithms.* 1970, Computer Journal, Vol. 13, pp. 317–322.

Forgy, E., *Cluster analysis of multivariate data: Efficiency versus interpretability of classification*. 1965, Biometrics, Vol. 21, pp. 768-780.

Foster, I.; Kesselman, C.; *The grid: blueprint for a new computing infrastructure*. 1998, The Elsevier Series in Grid Computing, ISBN 1-55860-933-4.

Foster, I.; Zhao, Y.; Raicu, I.; Lu, S.; *Cloud Computing and Grid Computing 360-Degree Compared*. 2008, IEEE Grid Computing Environments (GCE08), co-located with IEEE/ACM Supercomputing 2008.

Galton, F. 1877, *Typical laws of heredity*, Nature 15.

Garofalo, M.; *Seminario di tecnologie Web*. 2010, Corso di Tecnologie Astronomiche, Corso di Laurea Magistrale in Astrofisica e Scienze dello Spazio, Facoltà di Scienze, Università degli Studi di Napoli Federico II, Anno Accademico 2009/10.

Goldfarb, D., A *Family of Variable Metric Updates Derived by Variational Means.* 1970, Mathematics of Computation, Vol. 24, pp. 23–26.

Golub, G.H.; Ye, Q., *Inexact Preconditioned Conjugate Gradient Method with Inner-Outer Iteration.* 1999, SIAM Journal of Scientific Computation, Vol. 21, pp. 1305-1320.

Genova, F.; Rixon, G.; Ochsenbein, F.; Page, C.G., *Interoperability of archives in the VO*, *Proceedings of SPIE Conference Virtual Observatories*, Alexander S. Szalay Editor, Vol. 4846, pp.20-26, 2002.

Ghahramani, Z., Unsupervised Learning. Bousquet, O., Raetsch, G. and von Luxburg, U. (eds), 2004, *Advanced Lectures on Machine Learning*, Springer-Verlag, LNAI 3176.

Goldstein, M., *Swing model filtering using filter objects to reinterpret data and state models*, 2001, available at http://www-106.ibm.com/developerworks/java/library/j-filters/.

Gould, S.J.; *The Structure of Evolutionary Theory*, 2002, Harvard University Press.

Guenther, R.; Radebaugh, J., *Understanding Metadata*. 2004, National Information Standards Organization (NISO) Press, Bethesda MD, USA.

Gustafson J. L.; *Reevaluating Amdahl's Law*. 1988, Communications of the ACM, 31(5), pp. 532-533.

Guyon, I.; Elisseeff, A., 2003, *An Introduction to Variable and Feature Selection*, Journal of Machine Learning Research, Vol. 3, pp. 1157-1182.

Guyon, I.; Elisseeff, A. *In Feature Extraction*, Foundations and Applications, Guyon, I.; Gunn, S.; Nikravesh, M.; Zadeh, L. A. Editors; Series: Studies in Fuzziness and Soft Computing, Springer, 2006, Vol. 207.

Han, J.; Kamber, M., *Data Mining*. 2001, Morgan Kaufmann Publishers.

Harris, M.J.; *Real-Time Cloud Simulation and Rendering*. 2003, University of North Carolina Technical Report #TR03-040.

Hartigan, J.; Wong, M., *Algorithm AS136: A k-means clustering algorithm*. 1979, Applied Statistics, Vol. 28, pp. 100-108.

Hastie, T.; Tibshirani, R.; Friedman, J.; Franklin, J., *The elements of statistical learning: data mining, inference and prediction*. The Mathematical Intelligencer, 2005, Springer New York, Vol. 27, pp. 83-85.

Haykin, S., 1998, *Neural Networks - A Comprehensive Foundation* (2nd. ed.). Prentice-Hall, Upper Saddle River, NJ USA.

Heaton, J., *Applying Multithreading to Resilient Propagation and Backpropagation*. 2009, Heaton Research Inc., http://www.heatonresearch.com/encog/mprop/compare.html.

Hey, T.; Tansley, S.; Tolle, K., *The Fourth Paradigm: Data-Intensive Scientific Discovery;* ISBN-10: 0982544200, 2009; Microsoft Research, Redmond Washington, USA, 2009.

Hoberock, J.; N. Bell, *Thrust: A parallel template library*, 2010, available on line at http://code.google.com/ p/thrust/Holland, J.; *Adaptation in Natural and Artificial Systems*; The MIT Press, 1975.

Hyafil, L.; Rivest, R.L., *Constructing Optimal Binary Decision Trees is NP-complete.* 1976, Information Processing Letters, Vol. 5, pp. 15–17.

Inmon, B., *Building the Data Warehouse*. 1992. John Wiley and Sons. ISBN 0471569607.

Jacobs, R.A., *Increased rates of convergence through learning rate adaptation*. 1988, Neural Networks, Vol. 1, pp. 295–307.

Jain, A.; Dubes, R., *Algorithms for Clustering Data*. 1988, Prentice-Hall, Englewood Cliffs, NJ.

Jain, A.K.; Murty, M.N.; Flynn, P.J., *Data Clustering: A Review*, 1999, ACM Computing Surveys, Vol. 31, No. 3, pp. 264-323.

Kaelbling, A.; *Associative reinforcement learning: Functions in k-dnf*. 1994, Machine Learning, 15(3):279–298.

Kaufman, L.; Rousseeuw, P., *Finding Groups in Data: An Introduction to Cluster Analysis.* 1990, John Wiley and Sons, New York, NY.

Kirk, D. B.; Hwu, W.; *Programming Massively Parallel Processor, A Hands-on Approach*. 2010, Morgan Kaufmann Publishers, ISBN 0123814723.

Kohavi, R., *A study of cross-validation and bootstrap for accuracy estimation and model selection.* 1995, Proceedings of the Fourteenth International Joint Conference on Artificial Intelligence, Morgan Kaufmann Editions, San Mateo, Vol. 2, pp. 1137–1143.

Kohavi, R.; Provost, F., *Glossary of Terms*. 1998, In Editorial for the Special Issue on Applications of Machine Learning and the Knowledge Discovery Process, Machine Learning, Vol. 30, pp. 2-3.

Kohonen, T., *Self-Organizing Maps*. 2007, Springer, Heidelberg, Second ed., Vol. 30.

Kotsiantis, S. B., *Supervised Machine Learning: A Review of Classification Techniques*, Proceeding of the 2007 conference on Emerging Artificial Intelligence Applications in Computer Engineering, IOS Press Amsterdam, The Netherlands, 2007, Vol. 160, pp. 3-24.

Krauter, K.; Buyya, R.; Maheswaran, M.; A Taxonomy and Survey of Grid Resource Management System for Distributed Computing. 2002, Software Practice and Experience, 32(2):135-- 164.

LeBlanc, M.; Tibshirani, R., *Adaptive principal surfaces*, 1994, Journal of the American Statistical Association, vol. 89, pp. 53–64.

Lehmann, E. L.; Casella, G., *Theory of Point Estimation*. 1998, (2nd ed.), Springer, New York NY.

Lindeberg, T., *Feature detection with automatic scale selection*, 1998, International Journal of Computer Vision 30 (2): pp. 77–116.

Lindeberg, T., *Edge detection, in Encyclopedia of Mathematics*, M. Hazewinkel (editor), 2001, Kluwer/Springer, ISBN 1402006098.

Mattson, T. G.; Sanders, B. A.; Massingill, B. L.; Patterns of parallel programming. 2004, Upper Saddl and River, NJ: Addison -Wesley page. 21.

McLachlan, G.; Basford, K., *Mixture Models: Inference and Applications to Clustering.* 1988, Marcel Dekker ed., New York, NY.

McCulloch, W. S.; Pitts, W. H., *A logical calculus of the ideas immanent in nervous activity*. 1943, Bulletin of Mathematical Biophysics, Vol. 5, pp. 115-133.

Menard, S. W. 2001. *Applied logistic regression analysis*, Sage University Papers Series on Quantitative Applications in the Social Sciences, Thousand Oaks, CA, Vol. 106.

Meng Joo, E.; Fan, L.; *Genetic algorithms for MLP neural network parameters optimization*. 2009, in Control and Decision Conference, Guilin, China, 3653-3658.

Michalewicz, Z., *Genetic Algorithm +Data Structures = Evolution Programs*. 1996, Third ed., Springer-Verlag New York.

Mitchell, M., *An Introduction to Genetic Algorithms*. 1998, The MIT Press, Cambridge MA.

Moore, G. E. 1965, *Cramming more components onto integrated circuits.* Electronics Magazine, Vol. 38, Number 8.

Mosteller F.; Turkey J.W., *Data analysis, including statistics*. In Handbook of Social Psychology. Addison-Wesley, Reading, MA, 1968.

Murtagh, F., *Clustering in massive data sets*. 2002, Handbook of massive data sets, Kluwer Academic Publishers Norwell, MA USA.

Neapolitan, R. E., *Learning Bayesian Networks*, 2003. Prentice Hall, New York USA, ISBN-13 978-0130125347.

Nocedal, J., *Updating Quasi-Newton Matrices with Limited Storage*. 1980, Mathematics of Computation, Vol. 35, pp. 773–782.

Nocedal, J.; Wright, S. J., *Numerical optimization*. Springer Verlag, New York, NY, 1999.

NVIDIA Corporation, *CUDA C Best Practices Guide v4.0*. NVIDIA Corporation, Santa Clara, CA, 2011. Owens, J.D.; Houston, M.; Luebke, D.; Green, S.; Stone, J.E.; Phillips, J.C.; *GPU Computing*. 2008, Proceedings of the IEEE, vol. 96, No. 5, pp. 879–899.

Paliouras, G.; *Scalability of Machine Learning Algorithms*. 1993, M. Sc. Thesis, University of Manchester.

Park, J. M.; Lu, Y., *Edge detection in grayscale, color, and range images*, *in B. W. Wah* (editor) Encyclopedia of Computer Science and Engineering, 2008, doi 10.1002/9780470050118.ecse603.

Pasian, F.; Ameglio, S.; Becciani, U.; Borgani, S.; Gheller, C.; Manna, V.; Manzato, P.; Marseglia, L.; Smareglia, R.; Taffoni, G., *Interoperability and integration of theoretical data in the Virtual Observatory*. 2007, Highlights of Astronomy, IAU XXVI General Assembly, Vol. 14, p.632.

Pearl, J., Bayesian Networks: *A Model of Self-Activated Memory for Evidential Reasoning*, 1985. Proceedings of the 7th Conference of the Cognitive Science Society, University of California, Irvine, CA. pp. 329–334.

Phansalkar, V.V.; Sastry, P.S., Analysis of the back-propagation algorithm with momentum. 1994, IEEE Transactions on Neural Networks, Vol. 5, Issue 3, pp. 505-506.

Pratt, W. K., *Digital Image Processing*, 4th Edition, 2007, John Wiley & Sons Eds., Los Altos, California.

Press, W.H.; Teukolsky, S.A.; Vetterling, W.T.; Flannery, B.P., Markov Models and Hidden Markov Modeling. 2007, *Numerical Recipes: The Art of Scientific Computing* (3rd ed.), Section 16.3, Cambridge University Press, New York NY.

Provost, F.; Fawcett, T.; Kohavi, R., *The Case Against Accuracy Estimation for Comparing Induction Algorithms*, Proceedings of the 15th International Conference on Machine Learning, 1998, Morgan Kaufmann. pp. 445-553.

Rajaraman, A.; Ullmann, J.D.; *Mining of Massive Data Sets*. 2010, available on line at http://infolab.stanford.edu/~ullman/mmds.html.

Repici, J., (2010), *How To: The Comma Separated Value (CSV) File Format*. 2010, Creativyst Inc., http://www.creativyst.com/Doc/Articles/CSV/CSV01.htm

Ripley, B.D., *Statistical Data Mining*, 2002, Springer-Verlag, New York

Rosenblatt, F., *The Perceptron - a perceiving and recognizing automaton*. 1957, Report 85-460-1, Cornell Aeronautical Laboratory.

Rosendahl, S.; *Presentation for T-106.5800*. 2010, Seminar on Software Techniques.

Rubinstein, R.Y.; Kroese, D.P., *The Cross-Entropy Method: A Unified Approach to Combinatorial Optimization, Monte-Carlo Simulation and Machine Learning*. 2004, Springer-Verlag, New York NY.

Ruckstuhl, A.F.; Welsh, A.H., *Reference Bands for Nonparametrically Estimated Link Functions*. 1999, Journal of Computational and Graphical Statistics, Vol. 8, Nr. 4, pp. 699-714.

Rumelhart, D.; Hinton, G.; and Williams, R., *Learning internal representations by error propagation*. 1986, In Parallel Distributed Processing, MIT Press, Cambridge, MA, chapter 8.

Sadashiv, N.; Dilip Kumar, S.M.; Cluster, Grid and Cloud Computing: A Detailed Comparison. 2011, Proceedings of The 6th International Conference on Computer Science & Education (ICCSE 2011), August 3-5, SuperStar Virgo, Singapore, pg. 477-482.

Samet, H., 2006, *Foundations of Multidimensional and Metric Data Structures*. Morgan Kaufmann, San Francisco, USA. ISBN 0123694469.

Selim, S. Z.; Ismail, M. A., K-Means-Type Algorithms: *A Generalized Convergence Theorem and Characterization of Local Optimality*, IEEE Transactions on Pattern Analysis and Machine Intelligence, 1984, Vol. 6, Issue 1, IEEE Publishing, pp. 81-87.

Shadbolt, N.; Hall, W.; Berners-Lee, T.; *The Semantic Web Revisited*, IEEE Intelligent Systems, vol. 21, no. 3, pp. 96–101, 2006, doi: 10.1109/MIS.2006.62.

Shanno, D. F., *Conditioning of quasi-Newton methods for function minimization.* 1970, Mathematics of Computation, Vol. 24, pp. 647–656.

Shapiro, L. G.; Stockman, G. C., *Computer Vision*, 2001, New Jersey, Prentice-Hall, ISBN 0-13-030796-3, pp. 279-325.

Sorenson, H. W., *Parameter estimation: principles and problems*. 1980, M. Dekker Editor, Control and systems theory, Vol. 9, New York.

Stepanov A.; Lee M., *The Standard Template Library*, HP Laboratories Technical Report 95-11(R.1), November 1995.

Sutter, H.; The Free Lunch Is *Over: A Fundamental Turn Toward Concurrency in Software*, Dr. Dobb's Journal, 30(3), March 2005.

Sutton, R. S.; Barto A. G., *Reinforcement Learning: An Introduction*. 1998, The MIT Press, Cambridge, MA.

Taylor, I.J.; Deelman, E.; Gannon, D. B.; Shields, M. Eds., *Workflows for e-Science: Scientific Workflows for Grids*. London: Springer, 2007.

Tung, A.K.H.; NG, R.T.; Lakshmanan, L.V.S.; Han, J., *Constraint-Based Clustering in Large Databases*. 2001, In Proceedings of the 8th ICDT, London, UK.

Vapnik, V.N., *The Nature of Statistical Learning Theory*, 1995, Springer.

Vapnik, V. N., *Statistical Learning Theory*, 1998, John Wiley and Sons, New York.

Vetterling, T.; Flannery, B.P., *Conjugate Gradients Methods in Multidimensions*. 1992, Numerical Recipes in C - The Art of Scientific Computing, W. H. Press and S. A. Teukolsky Eds, Cambridge University Press; 2nd edition.

Viega, J; *Cloud Computing and the Common Man*. 2009, Computer, vol.42, no.8, pp.106-108, doi: 10.1109/MC.2009.252.

Vogl, T. P.; Mangis, J. K.; Rigler, A. K.; Zink, W. T.; Alkon, D. L., *Accelerating the convergence of the back-propagation method*. 1988, Biological Cybernetics, Vol. 59, pp. 257-263.

von Neumann, J., *First Draft of a Report on the EDVAC*. 1945.

Zahn, C. T., *Graph-theoretical methods for detecting and describing gestalt clusters, 1971, IEEE Transactions on Computers*, Vol. 20, No. 1, pp. 68-86.

Zhang, S.; He, Z; Implementation of Parallel Genetic Algorithm Based on CUDA. 209, Z. Cai et al. (Eds.): ISICA 2009, LNCS 5821, pp. 24-30, Springer-Verlag Berlin Heidelberg.

Weigend, A.S.; Mangeas, M.; Srivastava, A.N., *Nonlinear gated experts for time series: discovering regimes and avoiding overfitting*, 1995, International Journal of Neural Systems, pp.373-399.

Wells, D.C.; Greisen, E.W.; Harten, R.H., FITS: a *Flexible Image transport System.* 1981, Astronomy & Astrophysics Supplement Series, Vol. 44, p. 363.

Witten, I.H.; Frank, E., Data *Mining: Practical machine learning tools and techniques*. 2005, 2nd Edition, Morgan Kaufmann, San Francisco, USA.