Synopsis of the PhD Thesis - Network Computations in Artificial Intelligence*

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***Abstract*—Traditionally science is done using the reductionism paradigm. Artificial intelligence does not make an exception and it follows the same strategy. At the same time, network science tries to study complex systems as a whole. This synopsis presents my PhD thesis which takes an alternative approach to the reductionism strategy, with the aim to advance both fields, advocating that major breakthroughs can be made when these two are combined. The thesis illustrates this bidirectional relation by: (1) proposing a new method which uses artificial intelligence to improve network science algorithms (i.e. a new centrality metric which computes fully decentralized the nodes and links importance, on the polylogarithmic scale with respect to the number of nodes in the network); and (2) proposing two methods which take inspiration from network science to improve artificial intelligence algorithms (e.g. quadratic acceleration in terms of memory requirements and computational speed of artificial neural network fully connected layers during both, training and inference).**

***Index Terms*—network science, complex networks, artificial intelligence, machine learning, artificial neural networks, deep learning, evolutionary algorithms, communication networks**

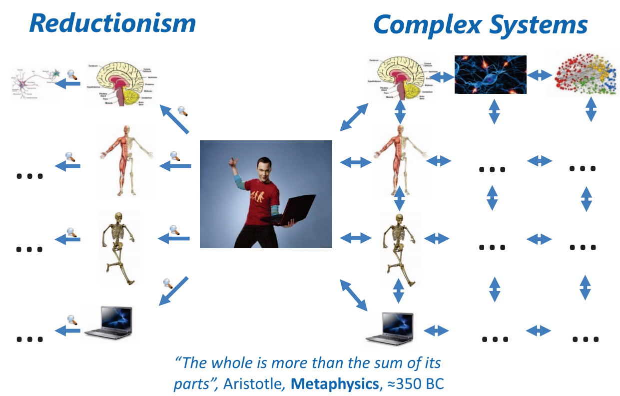

Fig. 1. Illustration of the reductionism and complex systems paradigms. It may be observed that while in the reductionism paradigm the main idea is to zoom in onto the various components of a system, the main emphasis in the complex systems paradigm is on unveiling connections among the various components and grasping the overall system behavior.

I. Introduction

Most of the science done throughout the human evolution uses the traditional reductionism paradigm, which attempts to explain the behavior of any type of system by zooming in on its constituent elements [1] and by summing their behavior. Consequently, nowadays we have an abundance of specializations and specialized people but few scientist study complex systems, which are in fact all around us. In my work, I do not claim reductionism to be wrong. On the contrary, it has been the basis of scientific advances throughout centuries of methodic investigation. Yet, my ambition is to understand the hidden properties that underlie complexity.

The limitations of reductionism were hinted millenniums ago by the ancient Greeks, Aristotle wrote in Metaphysics that *"The whole is more than the sum of its parts"*. At a first thought, the whole should be the sum of its parts. Still, some times we do not know all the parts and, in many cases, it may even be difficult to identify all those parts, let alone their mutual interdependencies. For instance, think about the gravitational waves. Gravity was first postulated by Isaac Newton in the 17^{th} century. Yet, the gravitational waves could have not considered in his theory, since that would have assumed that physical interactions propagate at infinite speed. Still, it was not until more than two centuries later, that Albert Einstein has intuited and predicted the existence of gravitational waves [2]; and it took about another century of great technological advancements before the existence of gravitational waves was proven [3].

To overcome the limitations of reductionism, the 'complex systems' paradigm aims to study the systems and their mutual interactions as a whole, which requires a multidisciplinary research, as depicted in Figure 1. This approach was first pioneered by the Santa Fe institute [4].

A complete theory of complexity is very hard to devise, but Network Science (NS) offers many of the required mathematical tools (e.g. complex networks) necessary to overpass reductionism [5]. Complex networks are graphs with non-trivial topological features, which are typical in many real world systems from a variety of research fields (e.g. neuroscience, astrophysics, biology, epidemiology, social and communication networks) [6].

At the same time, while the NS community has been trying to use Artificial Intelligence (AI) techniques to solve various NS open questions, such as in [7], the AI community has largely ignored the latest findings in network science. We

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argue that AI tends to follow the principles of reductionism and that new breakthroughs will need to go beyond it. In this thesis, following our initial thoughts from [8], we explore the potential arising from combining NS with AI, with emphasis on artificial neural networks [9] and evolutionary computation [10]. We set out with two long term research goals: (1) to better understand the fundamental principles behind the world near us, which may be modeled in amazing structures of networks of networks at micro and macro-scale, from the vigintillions of interacting atoms in the observable universe to the billions of persons in a social network; and (2) to advance the artificial intelligence field. We believe that these will ultimately help improving the general well-being of the human society, which is increasingly dependent upon intelligent software in complex systems of systems.

The remainder of this paper is organized as follows. Section II presents background knowledge. Section III briefly introduces some of our novel network science and artificial intelligence approaches to solve real-world problems with a focus on communication networks. Section IV discusses some common issues in state-of-the-art networks algorithms, and details the research questions addressed in my dissertation [11]. Section V presents an outline of the main dissertation contributions (i.e. the core research chapters) and provides a guideline to the reader. Finally, Section VI concludes this synopsis and presents further research directions.

II. Background

Network science is the academic field which studies complex networks [6], [12]. Any real-world network formalized from a graph theoretical perspective is a complex network. For example, such networks can be found in many domains from technical to social ones, such as telecommunication networks [13], [14], transportation networks [15], biology [16], [17] (e.g. biological neural networks, protein interactions), neuroscience [18]–[20], astrophysics [21], artificial intelligence [22] (e.g. artificial neural networks), semantic networks, social networks [23], [24], to mention but a few. In the study of complex networks, network science uses knowledge from many academic fields, such as mathematics (e.g. graph theory), physics (e.g. statistical mechanics), statistics (e.g. inferential modeling), computer science (e.g. data visualization, data mining), sociology (e.g. social structure) and so on.

Artificial intelligence is a subfield of computer science, which uses the concept of software intelligent agents to incorporate intelligence into machines [25]. The main research directions addressed by artificial intelligence are, mainly, knowledge representation, perception, learning, reasoning, and planning. These are, in fact, inspired to corresponding human cognitive functions. In this thesis, we address in more details, two subfields of artificial intelligence, namely machine learning and evolutionary computations.

III. Real-world challenges and our solutions

In this section, we consider practical, real-world problems, which pose hard scientific challenges, explaining how we have addressed them - either through novel solutions or through novel application of existing methods. We briefly discuss communication networks problems and our solutions, while for our proposed solutions in other domains we refer the reader to the corresponding articles, i.e. ABAC policy mining from logs in computer security [26], what and how to transfer [27], [28] in transfer learning, human activity recognition [29] and 3D trajectories estimation [30] in computer vision, real-time energy disaggregation in buildings [31] and on-line building energy optimization [32] in smart grids [33], [34].

A. Wireless sensor networks

With the emergence of sensors with wireless capability, most of current sensor networks consist of a collection of wirelessly interconnected units, each of them with embedded sensing, computing and communication capabilities [35]. Such sensor networks are referred to as Wireless Sensor Networks (WSNs) [36]. Due to their versatility, WSNs have been employed in a wide range of sensing and control applications, such as smart traffic control, environmental monitoring, security surveillance, and health-care [37]. As a consequence of cost, energy and spectrum constraints [38] sensors are prone to failure (hardware and transmission), as well as to data corruption. A typical approach to tackle these issues is through smart autonomic methods [39]–[42].

1) Redundancy reduction in WSN: The dense, unpredictable deployment of sensors leads to substantial data and networks [43]. In these situations, identifying the redundant sources and connections can save considerable resources (energy, communication spectrum, data processing and storage). In turn, this can extend the network life-time and scale [44], [45]. Redundancy reduction requires that the network stays fully connected to let the flow of information pass between any communication points.

In the scope of these arguments, in [46], we take advantage of the latest theoretical advances in complex networks, introducing a method that simplifies network topology based on centralized centrality metrics computations [6]. The method detects the redundant network elements to allow switching them off safely, without loss in connectivity. The experiments performed on a wide variety of network topologies with different sizes (e.g. number of nodes and links), using different centralized centrality metrics, validate our approach and recommend it as a solution for the automatic control of WSNs topologies during the exploitation phase of such networks to optimize, for instance, their life time.

2) Predictive power control in WSN: Besides that, prompt actions are necessary to achieve dependable communications and meet quality of service requirements in WSNs. To this end, the reactive algorithms used in the literature and standards, both centralized and distributed ones, are too slow and prone to cascading failures, instability and sub-optimality. In [47] we explore the predictive power of machine learning to better exploit the local information available in the WSN nodes and make sense of global trends. We aimed at predicting the configuration values that lead to network stability. We adopted

Q-learning, a reinforcement learning algorithm, to train WSNs to proactively start adapting in face of changing network conditions, acting on the available transmission power levels. The results demonstrate that smart nodes lead to better network performance with the aid of simple reinforcement learning.

B. Quality of experience

Quality of Experience (QoE) [48] aims at assessing the quality perceived by a user, while experiencing a service (e.g. video streaming services, web browsing, phone or video calls, server based enterprise software at the work environment and so on). Even though QoE is human centric, in general, due to the exponential increase of services, it is not practical to employ humans to assess the services quality. Thus, objective computational methods capable to assess the quality of those services such as humans do are needed [39].

1) Objective image quality assessment: Objectively measuring the quality degradation of images yielded by various impairments of the communication networks during a service is a difficult task, as there is often no original images to be used for direct comparisons. To address this problem, in [49] we proposed a novel reduced-reference QoE method, dubbed Restricted Boltzmann Machine Similarity Measure (RBMSim), that measures the quality degradation of 2D images, without requiring the original images for comparisons. Moreover, in [50] we take this work further, proposing a new reduced-reference QoE method to measure the quality degradation of 3D images using factored third order restricted Boltzmann machines [51], dubbed Q3D-RBM. What is interesting is that both, RBMSim and Q3D-RBM, perform just unsupervised learning taking advantage of RBM performance as density estimator. So, they do not need the ground truth, this being an important advantage for quality of experience methods. The experiments performed on benchmark datasets demonstrate that both methods achieve a similar performance to full reference objective metrics when benchmarked with subjective studies.

2) Objective video quality assessment: For obvious reasons, video quality assessment, is more difficult and more important than image quality assessment [52], [53]. In [54]–[58] we take further our work on images, proposing new no-reference and reduced-reference QoE methods to assess the quality degradation suffered by videos during streaming services. We use various models of artificial neural networks, from restricted Boltzmann machines to deep neural networks, using both unsupervised and supervised learning. The results show that, in general, the artificial neural networks used achieve very good performance, comparable with state-of-the-art objective full-reference metrics for video quality assessment, while not requiring the original videos for comparisons.

3) Objective quality of experience in enterprise and working environments: While most of the QoE studies aim at understanding the QoE impact of waiting times in controlled laboratories or in the user's domestic environment, the enterprise and working environments have been largely ignored. This happens due to the IT environment, which is highly complex and hard to analyze, and incurs high costs. In [59], by using a non-intrusive application monitoring of response times and subjective user ratings on the perceived application, we employ deep neural networks and other machine learning models to estimate the users QoE. The results show that we can successfully build machine learning models to estimate the QoE of specific users, but do not allow us to derive a generic model for all users.

IV. Research questions and objective

Following the study of a range of real-world problems, as outlined in Section III, we realized the enormous potential of both network science and machine learning. In all cases, scalability was the key limiting factors. With the aim of increasing the scalability bounds of various networks algorithms, we extrapolate a number of fundamental challenges, presented below as the *theoretical research questions* of my doctoral thesis [11]:

1) How to reduce the computational complexity when assessing the importance of all the elements of a complex network, i.e. nodes and links?
2) How to reduce the excessive memory requirements in artificial neural networks when they perform on-line learning?
3) How to reduce the computational complexity when training and exploiting artificial neural networks?

In the thesis, while trying to answer to these three research questions, we follow one single common *objective*:

- Any new method, which is to fulfill one of the three research questions above, will have to be comparably as accurate as its state-of-the-art counterparts.

V. Thesis main contributions and outline

Overall, we have discovered that the key to addressing the three research questions stated above lies in methods that combine artificial intelligence with network science methods, rather than employing them independently [8]. We elaborate on this claim through a selection of contributions included in Chapters 2, 3, 4, and 5 of the thesis [11], as summarized next.

A. Polylogarithmic centrality computations in complex networks - Chapter 2 [13], [60].

To compute the centrality of all elements (i.e. nodes and links) in a complex network is a difficult problem due to: (1) the difficulty of unveiling the hidden relations between all networks elements; (2) the computational time of state-of-the-art methods, which many times are not practical in real-world networks that are in excess of billions of nodes. Herein, we introduce a new class of fully decentralized stochastic methods, inspired by swarm intelligence and human behavior, to compute the centralities of all nodes and links simultaneously in a complex network. The basic idea is fairly simple. An homogeneous artificial system is overlaid over a complex network, which is a heterogeneous system (its topology gives its level of heterogeneity). After this, a gaming process starts, whereby the entities of the artificial system start interacting with the complex network. Over time, the artificial system evolves in such a way that will reveal the complex network features, specifically the nodes and links centrality. A proof of concept implementation of this algorithm can be found here[1]. The parallel time complexity of this approach is on the polylogarithmic scale with respect to the number of nodes in the network, while its accuracy is similar, and many times even better, than state-of-the-art centrality metrics. To give an impression on the magnitude of the computational problem at hand, if we were to consider one trillion Internet of Things devices (each one running the proposed protocol, over an unloaded network), and a transmission rate of 1 message per millisecond, then the centrality of all network elements (devices and the relations between them) would be computed in less than 22 seconds. As a comparison, by using other state-of-the-art centrality metrics for the same problem, one would need (perhaps) months to compute the results.

B. Generative Replay: towards memory-free online learning with ANNs - Chapter 3 [61].

Online learning with artificial neural networks is in many cases difficult due to the need of storing and relearning large amount of previous experiences. This limitation can be partially surpassed using a mechanism conceived in the early 1990s, named experience replay. Traditionally, experience replay can be applied in all types of ANN models to all machine learning paradigms (i.e. unsupervised, supervised, and reinforcement learning). Recently, it has contributed to improving the performance of deep reinforcement learning. Yet, its application to many practical settings is still limited by the excessive memory requirements, necessary to explicitly store previous observations. From a biological sense of memory, the human brain does not store all observations explicitly, but instead it dynamically generates approximate reconstructions of those experiences for recall. Inspired by this biological fact, to remedy the experience replay downside, we propose a novel approach dubbed generative replay. Generative replay uses the generative capabilities of restricted Boltzmann machines to generate approximations of past experiences, instead of recording them, as experience replay does. Thus, the RBM can be trained online, and does not require the system to store any of the observed data points. Furthermore, generative replay is a generic concept which may be used in combination with other types of generative artificial neural network models to serve dynamic approximations of past experiences to any ANN model that performs on-line learning.

C. Quadratic parameter reduction in artificial neural networks - Chapters 4 and 5 [22], [62]

Almost all of the artificial neural networks used nowadays contain fully connected layers, which have a quadratic number of connections with respect to the number of neurons. This type of fully connected layers contain the most of the neural network connections. Because the weight corresponding to each connection has to be carefully optimized during the learning process, this leads to increased computational requirements, proportionally to the number of connections that need to be optimized. Inspired by the fact that biological neural networks are sparse, and even more, they usually have small-world and scale-free topologies, in these two chapters we show that a striking amount of the connections from the fully connected layers of artificial neural networks is actually redundant. Furthermore, we demonstrate that we can safely decrease the number of connections from a quadratic relation to a linear relation, with respect to the number of neurons, at no decrease in accuracy (many times, even with an increase in accuracy). It is worth highlighting that the connections reduction is done in the design phase of the neural network, i.e. before training. In Chapter 4 [22], we use a fixed scale-free connectivity pattern. Furthermore, in Chapter 5 [62], we take this idea further and, starting with a random sparse connectivity pattern and adding an evolutionary process during the training phase of the ANN model, we are capable to reach even better performance. Our results show that it is possible to replace the fully connected layers in artificial neural networks with quadratically faster counterparts in both phases, training and exploitation. This type of sparse evolutionary ANN layers has low computational and memory requirements and may lead to the possibility of building ANN models in excess of billions of neurons. In the scope of these arguments, the proof of concept implementation[2] of this algorithm can build sparse ANN models with up to 1 million neurons on a standard laptop, this being way over current ANN possibilities.

To clarify, the above discussed theoretical advancements would have not been possible without having a complex systems approach, e.g. studying artificial intelligence and network science together and not separately as it is usually done using the reductionism paradigm. This paper is just a short overview of my thesis, while for the interested reader, an outlook of it is depicted in Figure 2.

VI. Conclusions and further work

To conclude, this thesis [11] addresses a range of topics around the common theme of *network efficiency*. We explore the fascinating opportunities that arise when AI is employed to master network complexity, and *vice versa*. The applicability of such fundamental concepts is vast, with the possibility to make impact on virtually any domain whereby problems can be modeled as networks. We have explored examples in communication networks [59], wireless sensor networks [13], [38], [46], [47], smart grids [31], [32], computer vision [29], [30], [63], computer security [26], transfer learning [27], [28], and multimedia quality of experience [49], [50], [54]–[58], [64], [65].

There is also enormous potential in employing scalable artificial neural networks onto other problems that cannot yet be tackled due to the scalability boundaries of current methods,

[1] https://github.com/dcmocanu/centrality-metrics-complex-networks

[2] https://github.com/dcmocanu/sparse-evolutionary-artificial-neural-networks

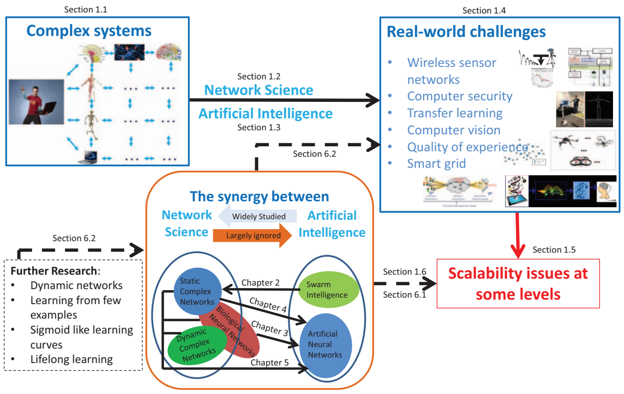

Fig. 2. Storyline of the PhD thesis "Network Computations in Artificial Intelligence" [11].

e.g. understanding of the brain, understanding of very high dimensional data, online learning in low-resources devices, etc.

Looking at the synergy between network science, artificial intelligence, and biological neural networks, we have been able to push the scalability bounds of various networks algorithms much beyond their state-of-the-art. Our combined approach to complexity and AI goes beyond the current methods, which tend to focus on either of the two, independently.

This research may be expanded in many directions. Let us group them into the two main categories of 'applied research' and 'fundamental research'. The applied research direction is straightforward and assumes applying the novel algorithms proposed in Section V to real-world challenges, as we described in Section III. The fundamental research direction could be furthered by continuing to explore the synergy between network science, artificial intelligence, and biological principles of nature. An interesting possibility would be to try to combine traditional AI techniques (i.e. knowledge representation, logic reasoning) with deep learning. This represents an important problem and an active research area, as highlighted by a recent paper [66]. One possibility to tackle it would be to follow our incipient approach, as proposed in [26], using restricted Boltzmann machines as density estimators for the inductive logic rules.

Another possibility, would be to study two of the most important challenges in artificial neural networks. The first one relates to the high number of examples that ANNs need to rely upon for learning. The second one is the slow learning curve of gradient based optimization methods. These do not follow the strategy of human learning, which have a much higher generalization power and can learn new concepts using just few labeled examples or even purely unsupervised [67]. Furthermore, the learning curve in humans is sigmodal, which is not the case of gradient based learning. Intuitively, one would hypothesize that if we could more accurately follow the laws of nature we would make new breakthroughs in machine learning, particularly in generalization capability, evolutionary and continuously learning. That would require achieving further insights into the dynamics of biological neural networks, looking from a network science perspective.

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