NEURAL NETWORKS AND ARTIFICIAL INTELLIGENCE

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Abstract. The pioneering methods and concepts developed by John Hopfield and Geoffrey Hinton have been instrumental in shaping the field of artificial neural networks (ANNs). In addition, Hinton played a leading role in the efforts to extend the methods to deep and dense ANNs. With their breakthroughs, which stand on the foundations of physical science, they have shown a completely new way for us to use computers to aid and to guide us in tackling many of the challenges in our society. Simply put, thanks to their work, Humanity now has a new item in its toolbox, which we can choose to use for good purposes. Machine learning based on ANNs is currently revolutionizing science, engineering, and daily life. The field is already on its way to enable breakthroughs toward building a sustainable society, e.g., by helping to identify new functional materials. How deep learning by ANNs will be used in the future depends on how we humans choose to use these incredibly potent tools, already present in many aspects of our lives. In this paper, we present a short survey on the work of the two Nobel laureates in the field of machine learning and neural networks. We present recent achievements in the field of machine learning and artificial intelligence. Moreover, we provide new results on machine learning through physics-informed neural networks.

Keywords: Neural networks, artificial intelligence, Nobel laureates, artificial neural networks, machine learning, physics-informed neural networks

1. NOBEL PRIZE FOR PHYSICS FOR NEURAL NETWORKS

The 2024 Nobel Laureates in Physics, John Hopfield and Geoffrey Hinton, use tools from physics to construct methods that help lay the foundations of today's machine learning. We quote the text of the Nobel Committee: "for foundational discoveries and inventions that enable machine learning with artificial neural networks". John Hopfield creates a structure that can remember and reconstruct information. Geoffrey Hinton invented a method that could independently discover properties of data, and that became important for modern artificial neural networks.

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Many people have wondered how computers can translate between languages, interpret images, and even have intelligent conversations. What is perhaps less well-known is that this type of technology has long been important to scientific research, including sorting and analyzing vast amounts of data. Machine learning has developed intensively over the past fifteen to twenty years and uses a structure called an artificial neural network. These days, when we talk about artificial intelligence (AI), this is often the type of technology we're referring to.

Although computers cannot think, machines can now mimic human brain functions such as memory and learning. This year's physics laureates have helped make that possible. Using fundamental concepts and methods from physics, they have developed technologies that use structures in networks to process information. With its roots in the 1940s, machine learning based on artificial neural networks has evolved over the past three decades as a versatile and powerful tool for both everyday and advanced scientific applications. With ANNs, the frontiers of physics are expanded both for phenomena of life and for computation.

2. HISTORICAL REMARKS

We will give some historical remarks on the development of machine learning.

The first electronically based computers appeared in the 1940s and were invented for military and scientific purposes. They were designed to perform calculations that were slow and time-consuming for scientists. In the 1950s, the opposite need emerged, namely to develop computers to do what humans and other mammals were good at – pattern recognition.

This AI-oriented goal was first approached by mathematicians and computer scientists who developed programs based on logical rules. This approach was proposed until the 1980s, but the computational resources required for accurate classifications, such as images, became impossible.

In parallel, efforts have been made to understand how biological systems solve the recognition problem. Already in 1943, Warren McCulloch and Walter Pitts [1], a neuroscientist and a logician, respectively, proposed a model of how neurons in the brain interact. In their model, a neuron forms a weighted sum of binary input signals from other neurons, which determines a binary output signal. Their development became a launching pad for later research in both biological and artificial neural networks. Another important early contribution came from psychologist Donald Hebb [2]. In 1949, Hebb proposed a mechanism for learning and memory in which the simultaneous and repeated activation of two neurons results in an increase in the strength of the synapse (connection) between them.

The natural neural network of the brain (Fig.1) is made up of living cells, neurons, with an advanced internal mechanism. They can send signals to each other through synapses. When we learn something, the connections between some neurons are

strengthened while others are weakened [3]. Artificial neural networks (Fig.2) are built from nodes that are encoded with a value. Nodes are connected to each other, and when the network is trained, the connections between nodes that are active at the same time are strengthened, otherwise, they are weakened.

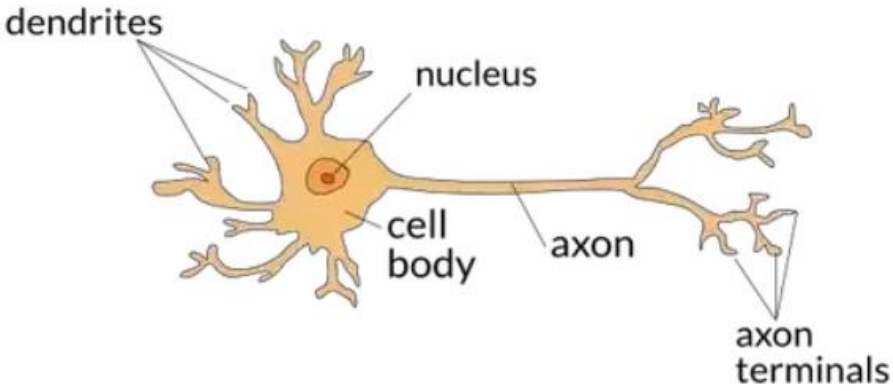

Fig. 1. A natural neural network.

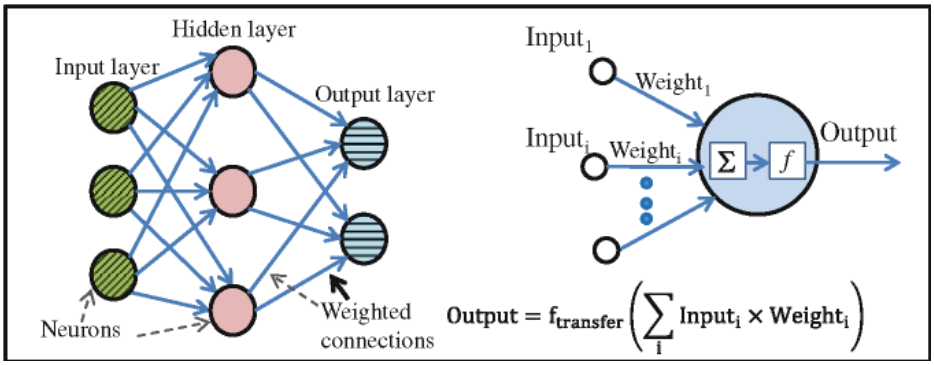

Fig. 2. Artificial neural network - abstract model.

In the field of ANN, two architectures of systems of interconnected nodes have been studied, "recurrent" (Fig. 3) and "feedforward" (Fig. 4) networks, where the former allows feedback interactions. A feed-forward network has input and output layers and may also contain additional layers of hidden nodes placed in between.

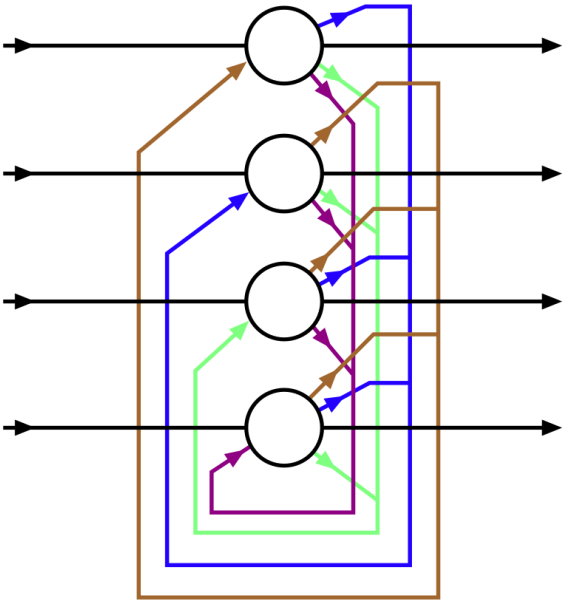

Fig. 3. Recurrent neural network

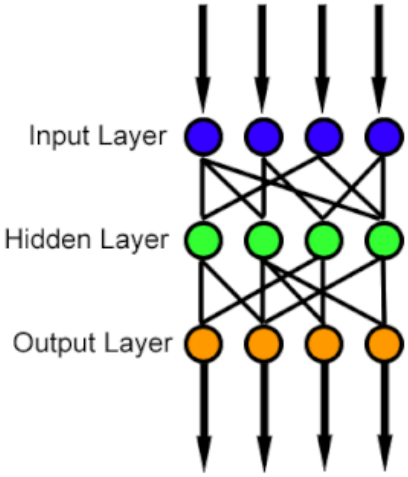

Fig. 4. Feedforward neural network

The 1960s and 1970s saw major breakthroughs in the fields of both recurrent and feedforward neural networks, leading to a rapid expansion of the ANN field [4-9].

3. NOBEL LAUREATES IN PHYSICS FOR 2024

John Hopfield, a theoretical physicist, is a famous scientist in biological physics. His major work in the 1970s investigated electron transfer between biomolecules [10] and error correction in biochemical reactions (kinetic correction) [11].

In 1980, Hopfield left his job at Princeton University, where his research interests took him outside the fields in which his physics colleagues were working, and moved to the other side of the continent. He accepted a professorship in chemistry and biology at the California Institute of Technology (Caltech) in Pasadena, Southern California. There, he had access to computing resources that he could use for free experiments and to develop his ideas about neural networks.

However, he did not abandon his foundation in physics, where he found inspiration for his understanding of how systems with very small components working together can lead to new and interesting phenomena. It is especially useful for him to become familiar with magnetic materials, which have special characteristics due to their atomic spin, a property that turns each atom into a small magnet. The spins of neighboring atoms influence each other; this may allow the formation of regions with spins in the same direction. He was able to create a network model of nodes and links using the physics that describes how materials evolve when spins affect each other.

In 1982, Hopfield published a dynamic model for associative memory based on a simple recurrent neural network [12]. Interrelated phenomena often occur in physical systems, such as domains in magnetic systems and vortices in fluid flow. Hopfield questions whether the occurrence of interconnected phenomena in large numbers of neurons can lead to "computational" properties. He answers this question using a neural network with N binary nodes s_i (0 or 1). The dynamics are asynchronous with threshold updates on individual nodes at random times. The new value of the node s_i is determined by the weighted sum of all other nodes,

$$h_i = \sum_{j \neq i}^{N} w_{ij} s_j,$$

and is set to s_i =1 if h_i>0, and s_i =0 otherwise (with threshold fixed to zero). The connections w_{ij} are symmetric and reflect pairwise correlations between nodes in stored memories, which is called Hebb's rule. The symmetry of the weights ensures stable dynamics. Stationary states are identified as memories distributed across N nodes in non-local storage. Furthermore, the network is characterized by an energy E,

$$E = -\int_{i<j} w_{ij} s_i s_j$$

which is a monotonically decreasing function under network dynamics. What is remarkable is that the connection between the world of physics as defined in the 1980s and the ANN is evident from these two equations. The first equation can be used to represent the molecular Weiss field (named after the French physicist Pierre Weiss), which describes how the atomic magnetic moments are arranged in a solid, and the latter is often used to estimate the energy of a magnetic configuration, e.g., in a ferromagnet. Hopfield was naturally aware of how these equations were used to describe magnetic materials.

When Hopfield published his paper on associative memory, Jeffrey Hinton was working at Carnegie Mellon University in Pittsburgh, USA. He previously studied experimental psychology and artificial intelligence in England and Scotland and was interested in whether machines could learn to process patterns in a human-like way, discovering their own categories to sort and interpret information. Together with his colleague Terrence Sejnowski [14], Hinton took Hopfield's network and extended it to build something new using ideas from statistical physics.

Statistical physics describes systems that consist of very similar elements (particles), such as molecules in a gas. It is difficult or impossible to track all the individual molecules in a gas, but it is possible to look at them together to determine the general properties of the gas, such as pressure or temperature. There are many potential ways for gas molecules to move through their volume at individual velocities and still result in the same collective properties.

The states in which individual components can coexist can be analyzed using statistical physics, and the probability of their occurrence is calculated. Some conditions are more likely than others; it depends on the amount of energy available, which is described in the Austrian physicist Ludwig Boltzmann's equation, derived at the end of the 19th century. Hinton's network uses this equation, and the method was published in 1985. under the impressive name "Boltzmann machine" [15].

4. MACHINE LEARNING

Machine learning, reorganized and recognized as its own field, started to flourish in the 1990s. The field changed its goal from achieving artificial intelligence to tackling solvable problems of a practical nature. It shifted focus away from the symbolic approaches it had inherited from AI and toward methods and models borrowed from statistics, fuzzy logic, and probability theory.

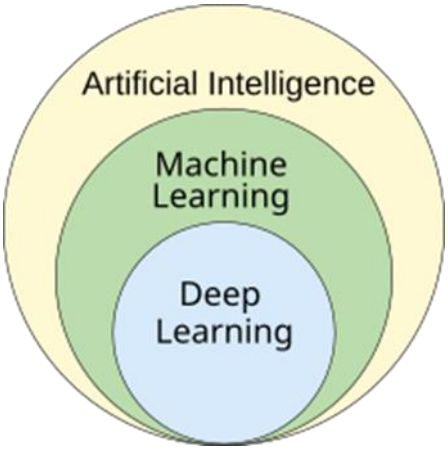

Fig. 5. Machine learning is a subfield of artificial intelligence.

As a scientific endeavor, machine learning grew out of the quest for artificial intelligence (AI). Artificial intelligence is the science and engineering of making intelligent machines was coined in 1956. In the early days of AI as an academic discipline, some researchers were interested in having machines learn from data. They attempted to approach the problem with various symbolic methods, as well as what were then termed neural networks, these were mostly perceptrons and other models that were later found to be reinventions of the generalized linear models. The first real results in AI had been achieved not in Expert systems- DENDRAL 1965, MYCIN 1972. The DENDRAL Project was one of the first large-scale programs to embody the strategy of using detailed, task-specific knowledge about a problem domain as a source of heuristics, and to seek generality through automating the acquisition of such knowledge. MYCIN was an early expert system, or artificial intelligence (AI) program, for treating blood infections. In 1972, work began on MYCIN at Stanford University in California. MYCIN would attempt to diagnose patients based on reported symptoms and medical test results. The program could request further information concerning the patient, as well as suggest additional laboratory tests, to arrive at a probable diagnosis, after which it would recommend a course of treatment.

British AI specialist David Hassabis and American chemist John M. Jumper were jointly awarded the Nobel Prize in Chemistry for their AI research contributions to protein structure prediction. Hassabis is working in the field of imagination, memory, and amnesia, he co-authored several influential papers published in Nature, Science, Neuron, etc. He developed a new theoretical account of the episodic memory system, identifying scene construction, the generation, and online maintenance of a complex and coherent scene as a key process underlying both memory recall and imagination.

A Boltzmann machine is typically used with two different types of knots. Information is fed to a group called visible nodes. The other nodes form a hidden layer.

The values and connections of hidden nodes also contribute to the energy of the network as a whole. The machine is controlled by applying a rule to update the values of the nodes one by one. Eventually, the machine will enter a state where the pattern of nodes may change, but the overall properties of the network remain the same. Each possible model will then have a certain probability, which is determined by the lattice energy according to the Boltzmann equation. When the machine stops, it has created a new pattern, making the Boltzmann machine an early example of a generative model.

Hopfield networks and Boltzmann machines are recurrent neural networks.

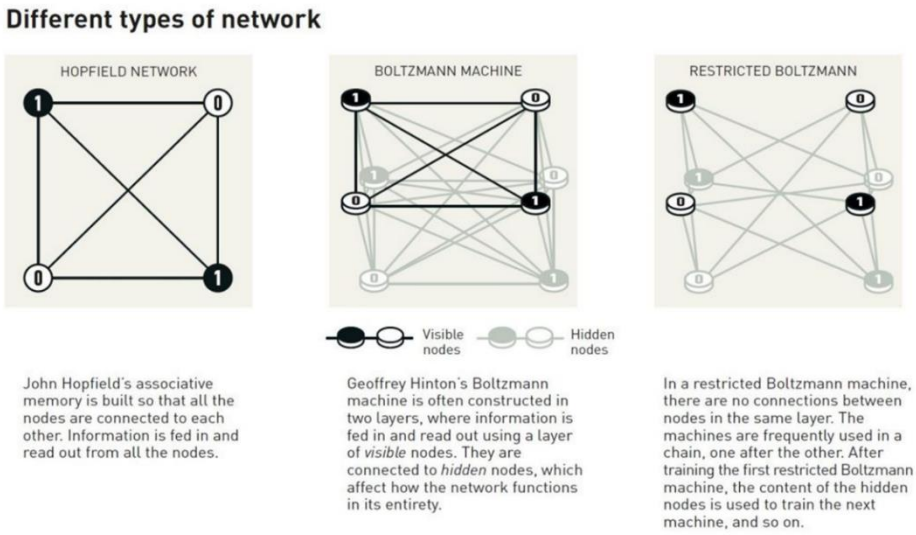

Fig. 6. Hopfield's neural network and Boltzmann's machine

In the 1990s, many researchers lost interest in artificial neural networks, but Hinton is one of those who continue to work in the field. It also helps usher in a new boom of exciting results; in 2006, he and his colleagues Simon Osindero, Yee Whye Teh, and Ruslan Salakhutdinov [18] developed a method for pretraining a network with a series of Boltzmann machines in layers, one on top of the other. This pre-training gives the connections in the network a better starting point, which optimizes its training for recognizing elements in pictures [15-19].

Through their work in the 1980s and beyond, John Hopfield and Geoffrey Hinton helped lay the groundwork for the machine learning revolution that began around 2010.

The developments we are witnessing now are made possible by access to vast amounts of data that can be used to train networks, and by massive increases in computing power. Modern artificial neural networks are often huge and made up of many

layers. These are called deep neural networks, and the way they are trained is called deep learning.

A quick look at Hopfield's 1982 paper on associative memory. [12] provides some perspective on this development. In it, he uses a network with 30 nodes. If all nodes are connected to each other, they have 435 connections. Nodes have their own values that have different strengths, and overall, there are fewer than 500 parameters to keep track of. He also tried a 100-node network, but that was too complicated given the computer he was using at the time. We can compare this to today's large language models, which are built as networks that can contain more than a trillion parameters.

Currently, many researchers are developing the application areas of machine learning. Which of these will be the most viable remains to be seen, while there are wide-ranging discussions about the ethical issues that accompany the development and use of this technology.

Since physics has contributed tools to the development of machine learning, it is interesting to see how physics, as a research field, also benefits from artificial neural networks. Machine learning has long been used in fields that may be familiar to us from previous Nobel Prizes in physics. Among them is the use of machine learning to sift through and process the vast amounts of data needed to discover the Higgs boson. Other applications include noise reduction in measurements of gravitational waves from colliding black holes or the search for exoplanets.

In recent years, this technology has also begun to be used to calculate and predict the properties of molecules and materials - for example, to calculate the structure of protein molecules that determines their function, or to determine which new versions of a material might have the best properties for use in more efficient solar cells.

5. MACHINE LEARNING THROUGH PHYSICS INFORMED NEURAL NETWORKS

Artificial intelligence based on physics-informed neural networks (PINN) represents a new scientific technique from machine learning for solving various tasks, modelling real processes. PINNs were introduced in 2017 as a new class of data-driven solvers in a two-part paper [21, 22,23] published in a merged version subsequently in 2019 [24]. Raisi et al. [24] introduce and illustrate the PINN approach for solving nonlinear differential equations, such as the Schrödinger, Burgers, and Allen-Cohn equations. They create physics-informed neural networks that can handle both tasks—the forward task of evaluating the solutions of the governing mathematical models, and the inverse task, where model parameters are learned from observable data.

PINNs have several advantages over conventional methods. They allow solutions to be differentiated using analytic gradients and provide an easy way to solve direct

and inverse problems using an optimization problem. In addition to solving differential equations (a forward problem), PINNs can be used to solve inverse problems such as characterizing data streams. PINNs' algorithms and codes allow for attacking high-order differential equations that are difficult for numerical simulations. Physically informed neural networks can address tasks that are described with little data.

PINNs can solve differential equations expressed in the most general form, such as:

$$\mathcal{F}(u(z),\gamma) = f(z), z \text{ in } \Omega$$

$$\mathcal{B}\big(u(z)\big) = g(z), z \text{ in } \partial\Omega \tag{1}$$

defined in the domain $\Omega \subset R^d$ with boundary $\partial\Omega, z := [x\_1, \cdots, x\_(d-1); t]$ is a vector with coordinates space-time, u is an unknown solution, γ are the parameters, f is a function defining the problem's data, $\mathcal{F}$ is a nonlinear differential operator. Finally, since the initial condition can actually be seen as a type of Dirichlet boundary condition on the space-time domain, it is possible to denote $\mathcal{B}$ as an operator specifying arbitrary initial or boundary conditions associated with the problem, and g as the boundary function. Indeed, the boundary conditions can be Dirichlet, Neumann, Robin, or periodic boundary conditions.

Equation (1) can describe many real processes, including both forward and inverse problems. The goal of a straight problem is to find the function u for each z, where γ there are certain parameters. In the case of the inverse problem, γ must also be determined from data. An operator-based mathematical formulation of equation (1) can be found in the work of Mishra and Molinaro [20].

In the PINN methodology, $u(z)$ is numerically predicted by a neural network parameterized by a set of parameters θ, which leads to an approximation

$$\hat{u}_\theta(z) \approx u(z)$$

where with $\hat{u}_\theta$ is denoted as the approximation with the neural network with respect to θ.

In this context, since both forward and inverse problems are analyzed in the same framework, given that PINNs can solve both problems, we will use θ to simultaneously represent a vector of all unknown parameters in the neural network of the initial model and the unknown parameters γ in the case of the inverse problem. The neural network must then learn to approximate the differential equations by finding the θ that defines the neural network by minimizing a loss function that depends on the differential equation (LF), the boundary conditions (LB), and possibly some known data (Ldata), all of which are adequately weighted:

$$\theta^* = arg\, min_\theta(\omega_{\mathcal{F}} L_{\mathcal{F}}(\theta) + \omega_{\mathcal{B}} L_{\mathcal{B}}(\theta) + \omega_d\, L_{data}(\theta)). \tag{2}$$

Figure 7 generalizes all structural elements of PINNs, which were discussed.

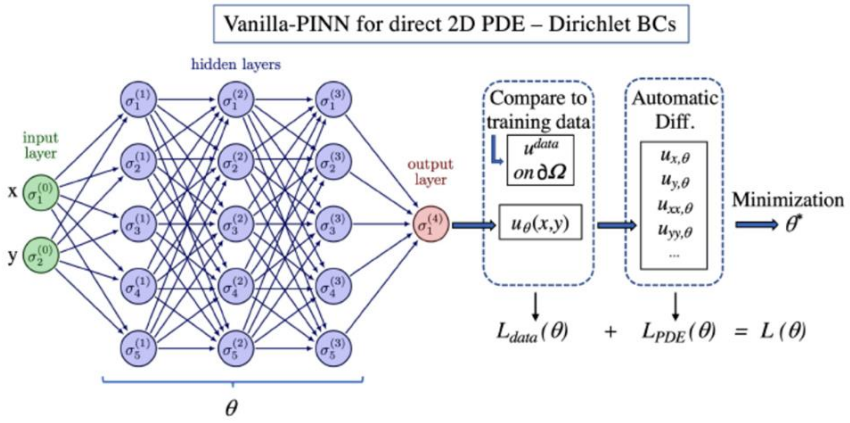

Fig. 7. Architecture of PINN.

Neural networks are a method in artificial intelligence that trains computers to process data in a way inspired by the human brain. The development in recent years of digital technologies for the collection of multidimensional huge data sets places new demands on the existing methods for their modeling, analysis, and structuring. Important for practice, on one hand, are the modifications of the existing theoretical algorithms and, along with that, the ways of their effective application in various processes.

Physics-informed neural networks (PINNs) were introduced to investigate nonlinear differential equations using machine learning and artificial intelligence approaches. Modern PINNs-based methods have advantages in optimization and automatic differentiation. They have the potential to address the following two challenges in a relatively simple and rapid way: 1). processing huge databases of numerical and observational data, and 2). Solving highly complex nonlinear models of real processes. In [25], PINN is applied to solve some nonlinear PDEs of mathematical physics.

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