Geometry-Based Deep Learning in the Natural Sciences

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Nature is composed of elements at various spatial scales, ranging from the atomic to the astronomical level. In general, human sensory experience is limited to the mid-range of these spatial scales, in that the scales which represent the world of the very small or very large are generally apart from our sensory experiences. Furthermore, the complexities of Nature and its underlying elements are not tractable nor easily recognized by the traditional forms of human reasoning. Instead, the natural and mathematical sciences have emerged to model the complexities of Nature, leading to knowledge of the physical world. This level of predictiveness far exceeds any mere visual representations as naively formed in the Mind. In particular, geometry has served an outsized role in the mathematical representations of Nature, such as in the explanation of the movement of planets across the night sky. Geometry not only provides a framework for knowledge of the myriad of natural processes, but also as a mechanism for the theoretical understanding of those natural processes not yet observed, leading to visualization, abstraction, and models with insight and explanatory power. Without these tools, human experience would be limited to sensory feedback, which reflects a very small fraction of the properties of objects that exist in the natural world. As a consequence, as taught during the times of antiquity, geometry is essential for forming knowledge and differentiating opinion from true belief. It not only provides a framework for understanding astronomy, classical mechanics, and relativistic physics, but also the morphological evolution of living organisms, along with the complexities of the cognitive systems. Geometry also has a role in the information sciences, where it has explanatory power in visualizing the flow, structure, and organization of information in a system. This role further impacts the explanations of the internals of deep learning systems as developed in the fields of computer science and engineering.

geometrical representation | cognitive process | mathematical model | artificial intelligence

Historical Perspective on Geometry

A modern view of the physical world, and likewise in the study of the natural sciences, is dependent on models. The ideal model is written in the precise and reliable language and symbols of mathematics, a practice that allows for theoretical study and generalizing of the physical processes of Nature. This is a predictive capability that leads to knowledge of the physical world that is outside human perceptual experience. The potentiality of mathematics was explored by the philosophers of antiquity, such as Pythagoras and the Pythagoreans in ancient Greece [1]. At this time, arithmetics and geometry were taught as foundational to subsequent instruction in astronomy and music [2]. The strength of this approach was fully realized in Ptolemy's Almagest, a literary work on the mathematical foundations for explaining the observations and motion of planets across the night sky [3]. His work depended on instruments and precise measurement. This practice led to astronomical charts that are capable of predicting a planet's position in the night sky. Ptolemy further applied these models as a guide so others could construct a device that corresponds to the design of today's planetariums [3].

Improvements in mathematics and instrumentation led to the early 17th century works of Galileo and his contributions to knowledge of the physical world, such as the geometry of motion, along with convincing evidence (Galileo, 1610) against the geocentric model, and in favor of the heliocentric model (Copernicus, 1543) of planetary motion [4][5].

By the end of the 17th century, Isaac Newton established classical mechanics by application of mathematical theory and empirical observation [6]. These mathematical models led to a newfound explanatory power on the behavior of objects as observed in the physical world. As observations improved over the subsequent centuries, mathematics and its symbols continued to develop and a language emerged for explanation of the physical processes outside our sensory experience, such as the world of the very large, as with the force of gravity as exerted on an astronomical-sized object, and the world of the very small, such as the atomic forces among the elemental forms of matter [7]. Many of these innovations were based on geometry as an abstract construction of the spatial context of the physical forces of Nature. These geometrical models were first based on three-dimensional space as defined by Euclid [8]: a space with zero curvature. By the 20th century, the physical world was becoming explained by models no longer constrained by zero curvature, such as Hermann Minkowski's model for a physical world where three-dimensional space and one-dimensional time were combined into a system with a single four-dimensional space–time [9].

The Explanatory Power of Geometry

These examples show that geometrical objects are descriptive of the properties and processes of Nature. They can also abstractly represent the flow of information, a kind of mechanical process. Geometry is a visual language with reliance on symbols for expression of conceptual knowledge. Therefore, the indescribable processes of Nature can now be visualized as objects of the Mind. This is not just a language as a sequence of symbols, but instead a visual description with the permanence and reliability of a mathematical language. Humans are limited in their capability in the perception of the physical world [10]. For example, the Mind is not capable of forming a visualization of spacetime dynamics as it truly exists in the physical world, but instead as a geometrical model—a mathematical representation that is in a conceptualizable format [11].

The spaces and manifolds of geometry are therefore observable in the Mind and as hypotheses unbounded by our limited conception of reality. This conception is limited by the range of the senses, a phenomenon that is essentially a product of the reflection of objects of the natural world, but not the objects in and of themselves [10][11]. In the case of "seeing" an object, such as a table or a chair, the object is not observed directly, but instead as a reflection of light that is received by an array of molecular sensors in the inner surface of the eye [10]. An outsized portion of the brain is dedicated to processing this information and constructing the percepts, leading to inaccuracies; but, moreover, these visualizations are constrained to a very narrow range of all possible forms of light, hence the reference to this spectrum as the range of “visible light”. Further, this limitation in perception is not a product of chance, but of necessity, as it overlaps with the light spectrum as emitted from the Sun and received at the surface of the Earth.

Geometrical description extends beyond the common objects of the physical world, to use in explanations on the flow of information, a phenomenon also dependent on physical processes [12]. An example is a graph-based description of information that flows between an interconnected system of computing devices. This graph is idealized as a fully connected network [13] (**Figure 1**). This representation of information and its flow further applies to the artificial neural networks (ANNs) of computer science, a graph consisting of nodes and connections [14]. While pseudocode may be used to describe an ANN, it is not a basis to form generalizations about them. However, the mathematical representations of ANNs, particularly those of geometry, lead to a model-based framework that is adapted for interpretability. Geometrical representations further provide a visualization on the properties of an idealized network, such as observed in a sparsely connected network [15].

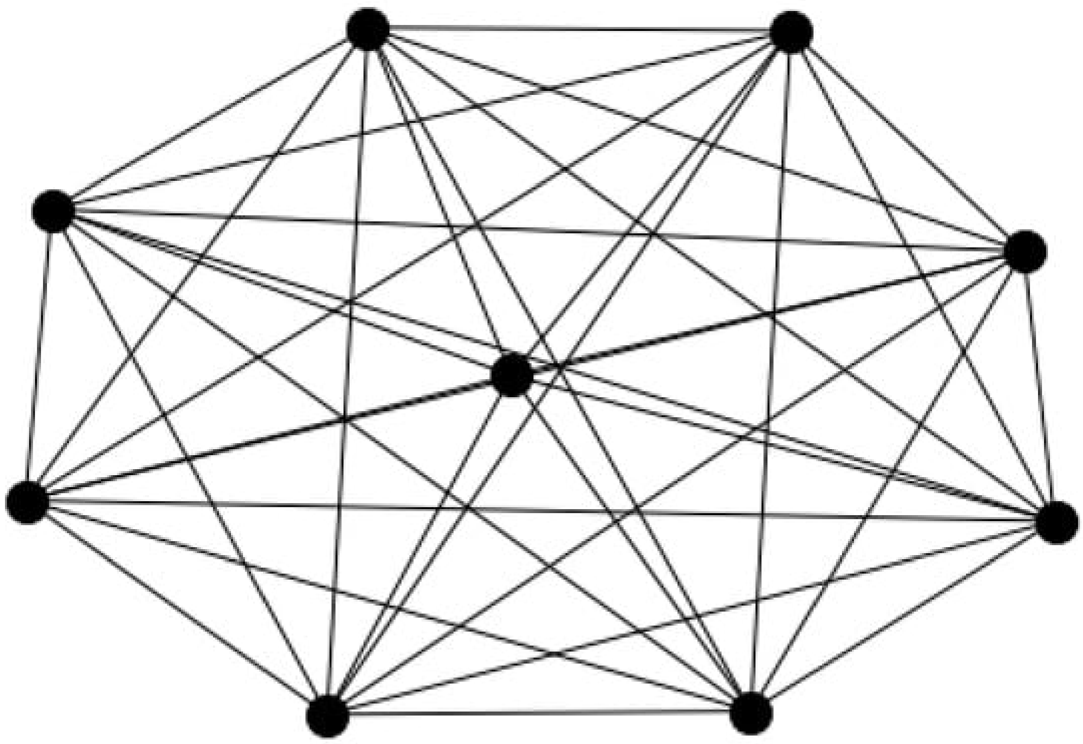

Figure 1. A fully connected network. Each node shares a connection with all other nodes. The number of connections in this network increases quadratically with an increase in the number of nodes. This expectation is identical to that which occurs in the attention mechanism of the transformer architecture of deep learning [16][17]. Furthermore, this leads to limits on the computation by a transformer. The cause of this limit may be referred to as a combinatorial explosion as there is a calculation at each edge, and, therefore, the number of calculations potentially exceeds that of an exponential growth rate. (Figure and legend reproduced from [13].)

In the literature of deep learning, the neural network layers are often presented in a visual format with the flow of information from module to module [16]. This is a similar practice to that which emerged in ecology and study of the large-scale ecological processes, a visualization of processes based on thermodynamics, leading to a paradigmatic shift, ranging from approaches to measuring the influence of microorganisms within an ecosystem to the study of the biogeochemical processes across the biosphere of the Earth [18].

Recent advances in deep learning include that of development of large language models as based on a transformer architecture [16][19]. Central to this architecture is an attention module, a variant of the attention mechanism for use in ANNs [20]. An insightful description of this module is shown as a series of modules [19], beginning from input to a module where the input is representable by a fully connected graph (**Figure 1**). Each connection of the graph is of equal weight. The transformer subsequently prunes edges that leads to a sparsely connected graph. Pure mathematics is also replete with examples of similar visual explanations of concepts, particularly in the foundational area of linear algebra and high-dimensional computation.

References

1. The Stanford Encyclopedia of Philosophy; Stanford University: Stanford, CA, USA, 2019; Available online: https://plato.stanford.edu/entries/pythagoreanism (accessed on 25 April 2023).
2. Proust, D. The Harmony of the Spheres from Pythagoras to Voyager. Proc. Int. Astron. Union 2009, 5, 358–367.
3. Murschel, A. The Structure and Function of Ptolemy’s Physical Hypotheses of Planetary Motion. J. Hist. Astron. 1995, 26, 33–61.
4. Van Helden, A. Galileo, telescopic astronomy, and the Copernican system. In Planetary Astronomy from the Renaissance to the Rise of Astrophysics; Taton, R., Wilson, C., Eds.; Cambridge University Press: Cambridge, UK, 1989.
5. Settle, T.B. An Experiment in the History of Science: With a simple but ingenious device Galileo could obtain relatively precise time measurements. Science 1961, 133, 19–23.
6. Truesdell, C. History of Classical Mechanics (Part I). Naturwissenschaften 1976, 63, 53–62.
7. Kleppner, D. A short history of atomic physics in the twentieth century. Rev. Mod. Phys. 1999, 71, S78.
8. Hartshorne, R. Geometry: Euclid and Beyond; Springer Science & Business Media: New York, NY, USA, 2013.
9. Arthur, R.T. Minkowski Spacetime and the Dimensions of the Present. Philos. Found. Phys. 2006, 1, 129–155.
10. Friedman, R. Themes of advanced information processing in the primate brain. AIMS Neurosci. 2020, 7, 373.

11. Waddell, W.W. The Parmenides of Plato; James Maclehose and Sons: Glasgow, UK, 1894.
12. Barrett, T.W. Conservation of information. Acta Acust. United Acust. 1972, 27, 44–47.
13. Friedman, R. Detecting Square Grid Structure in an Animal Neuronal Network. NeuroSci 2022, 3, 91–103.
14. Linial, N.; London, E.; Rabinovich, Y. The geometry of graphs and some of its algorithmic applications. Combinatorica 1995, 15, 215–245.
15. Goswami, S.; Murthy, C.A.; Das, A.K. Sparsity measure of a network graph: Gini index. Inf. Sci. 2018, 462, 16–39.
16. Vaswani, A.; Shazeer, N.; Parmar, N.; Uszkoreit, J.; Jones, L.; Gomez, A.N.; Kaiser, L.; Polosukhin, I. Attention is all you need. In Proceedings of the 31st Conference on Neural Information Processing System, Long Beach, CA, USA, 4–9 December 2017; pp. 5998–6008.
17. Chen, L.; Lu, K.; Rajeswaran, A.; Lee, K.; Grover, A.; Laskin, M.; Abbeel, P.; Srinivas, A.; Mordatch, I. Decision Transformer: Reinforcement Learning via Sequence Modeling. Adv. Neural Inf. Process. Syst. 2021, 34, 15084–15097.
18. Odum, E.P. Energy flow in ecosystems—A historical review. Am. Zool. 1968, 8, 11–18.
19. Hu, Y.; Buehler, M.J. Deep language models for interpretative and predictive materials science. APL Mach. Learn. 2023, 1, 010901.
20. Schmidhuber, J. Learning to Control Fast-Weight Memories: An Alternative to Dynamic Recurrent Networks. Neural Comput. 1992, 4, 131–139.