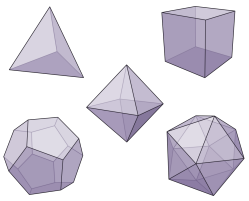
these architectures, a canonical mesh (of the body, face, or hand) was assumed to be known and the synthesis task consisted of regressing the 3D coordinates of the nodes (the embedding of the surface, using the jargon of differential geometry). Kulon et al. (2020) showed a hybrid pipeline for 3D hand pose estimation with an image CNN-based encoder and a geometric decoder. A demo of this system, developed in collaboration with a British startup company Ariel AI and presented at CVPR 2020, allowed to create realistic body avatars with fully articulated hands from video input on a mobile phone faster than real-time. Ariel AI was acquired by Snap in 2020, and at the time of writing its technology is used in Snap's augmented reality products.

Examples of complex 3D hand poses reconstructed from 2D images in the wild (Kulon et al., 2020).

7 Historic Perspective

"Symmetry, as wide or as narrow as you may define its meaning, is one idea by which man through the ages has tried to comprehend and create order, beauty, and perfection." This somewhat poetic definition of symmetry is given in the eponymous book of the great mathematician Hermann Weyl (2015), his *Schwanengesang* on the eve of retirement from the Institute for Advanced Study in Princeton. Weyl traces the special place symmetry has occupied in science and art to the ancient times, from Sumerian symmetric designs to the Pythagoreans who believed the circle to be perfect due to its rotational symmetry. Plato considered the five regular polyhedra bearing his name today so fundamental that they must be the basic building blocks shaping the material world. Yet, though Plato is credited with coining the term συμμετρία, which literally translates as 'same measure', he used it only vaguely to convey the beauty of proportion in art and harmony in music. It was the astronomer and mathematician Johannes Kepler to attempt the first rigorous analysis of the symmetric shape of water crystals. In his treatise ('On the Six-Cornered Snowflake'), he attributed the six-fold dihedral structure of snowflakes to hexagonal packing of particles – an idea that though preceded the clear understanding of how matter is formed, still holds today as the basis of crystallography (Ball, 2011).



The tetrahedron, cube, octahedron, dodecahedron, and icosahedron are called *Platonic solids*.

Fully titled *Strena, Seu De Nive Sexangula* ('New Year's gift, or on the Six-Cornered Snowflake') was, as suggested by the title, a small booklet sent by Kepler in 1611 as a Christmas gift to his patron and friend Johannes Matthäus Wackher von Wackenfels.

Symmetry in Mathematics and Physics In modern mathematics, symmetry is almost univocally expressed in the language of group theory. The origins of this theory are usually attributed to Évariste Galois, who coined

the term and used it to study solvability of polynomial equations in the 1830s. Two other names associated with group theory are those of Sophus Lie and Felix Klein, who met and worked fruitfully together for a period of time (Tobies, 2019). The former would develop the theory of continuous symmetries that today bears his name; the latter proclaimed group theory to be the organising principle of geometry in his Erlangen Program, which we mentioned in the beginning of this text. Riemannian geometry was explicitly excluded from Klein's unified geometric picture, and it took another fifty years before it was integrated, largely thanks to the work of Élie Cartan in the 1920s.

Emmy Noether, Klein's colleague in Göttingen, proved that every differentiable symmetry of the action of a physical system has a corresponding conservation law (Noether, 1918). In physics, it was a stunning result: beforehand, meticulous experimental observation was required to discover fundamental laws such as the conservation of energy, and even then, it was an empirical result not coming from anywhere. Noether's Theorem — "a guiding star to 20th and 21st century physics", in the words of the Nobel laureate Frank Wilczek — showed that the conservation of energy emerges from the translational symmetry of time, a rather intuitive idea that the results of an experiment should not depend on whether it is conducted today or tomorrow.

The symmetry associated with charge conservation is the global *gauge invariance* of the electromagnetic field, first appearing in Maxwell's formulation of electrodynamics (Maxwell, 1865); however, its importance initially remained unnoticed. The same Hermann Weyl who wrote so dithyrambically about symmetry is the one who first introduced the concept of gauge invariance in physics in the early 20th century, emphasizing its role as a principle from which electromagnetism can be *derived*. It took several decades until this fundamental principle — in its generalised form developed by Yang and Mills (1954) — proved successful in providing a unified framework to describe the quantum-mechanical behavior of electromagnetism and the weak and strong forces, finally culminating in the Standard Model that captures all the fundamental forces of nature but gravity. We can thus join another Nobel-winning physicist, Philip Anderson (1972), in concluding that "it is only slightly overstating the case to say that physics is the study of symmetry."

Weyl first conjectured (incorrectly) in 1919 that invariance under the change of scale or "gauge" was a local symmetry of electromagnetism. The term *gauge*, or *Eich* in German, was chosen by analogy to the various track gauges of railroads. After the development of quantum mechanics, Weyl (1929) modified the gauge choice by replacing the scale factor with a change of wave phase. See Straumann (1996).

Early Use of Symmetry in Machine Learning In machine learning and its applications to pattern recognition and computer vision, the importance of symmetry has long been recognised. Early work on designing equivariant feature detectors for pattern recognition was done by Amari (1978), Kanatani (2012), and Lenz (1990). In the neural networks literature, the famous Group Invariance Theorem for Perceptrons by Minsky and Papert (2017) puts fundamental limitations on the capabilities of (single-layer) perceptrons to learn invariants. This was one of the primary motivations for studying multi-layer architectures (Sejnowski et al., 1986; Shawe-Taylor, 1989, 1993), which ultimately led to deep learning.

Shun'ichi Amari is credited as the creator of the field of *information geometry* that applies Riemannian geometry models to probability. The main object studied by information geometry is a *statistical manifold*, where each point corresponds to a probability distribution.

In the neural network community, *Neocognitron* (Fukushima and Miyake, 1982) is credited as the first implementation of shift invariance in a neural network for "pattern recognition unaffected by shift in position". His solution came in the form of hierarchical neural network with local connectivity, drawing inspiration from the receptive fields discovered in the visual cortex by the neuroscientists David Hubel and Torsten Wiesel two decades earlier (Hubel and Wiesel, 1959). These ideas culminated in Convolutional Neural Networks in the seminal work of Yann LeCun and co-authors (LeCun et al., 1998). The first work to take a representation-theoretical view on invariant and equivariant neural networks was performed by Wood and Shawe-Taylor (1996), unfortunately rarely cited. More recent incarnations of these ideas include the works of Makadia et al. (2007); Esteves et al. (2020) and one of the authors of this text (Cohen and Welling, 2016).

This classical work was recognised by the Nobel Prize in Medicine in 1981, which Hubel and Wiesel shared with Roger Sperry.

Graph Neural Networks It is difficult to pinpoint exactly when the concept of Graph Neural Networks began to emerge—partly due to the fact that most of the early work did not place graphs as a first-class citizen, partly since GNNs became practical only in the late 2010s, and partly because this field emerged from the confluence of several research areas. That being said, early forms of graph neural networks can be traced back at least to the 1990s, with examples including Alessandro Sperduti's Labeling RAAM (Sperduti, 1994), the "backpropagation through structure" of Goller and Kuchler (1996), and adaptive processing of data structures (Sperduti and Starita, 1997; Frasconi et al., 1998). While these works were primarily concerned with operating over "structures" (often trees or directed acyclic graphs), many of the invariances preserved in their architectures are reminiscent of the GNNs more commonly in use today.

The first proper treatment of the processing of generic graph structures (and the coining of the term *"graph neural network"*) happened after the turn of the 21st century. Within the Artificial Intelligence lab at the Università degli Studi di Siena (Italy), papers led by Marco Gori and Franco Scarselli have proposed the first "GNN" (Gori et al., 2005; Scarselli et al., 2008). They relied on recurrent mechanisms, required the neural network parameters to specify *contraction mappings*, and thus computing node representations by searching for a fixed point—this in itself necessitated a special form of backpropagation (Almeida, 1990; Pineda, 1988) and did not depend on node features at all. All of the above issues were rectified by the Gated GNN (GGNN) model of Li et al. (2015). GGNNs brought many benefits of modern RNNs, such as gating mechanisms (Cho et al., 2014) and backpropagation through time, to the GNN model, and remain popular today.

Concurrently, Alessio Micheli had proposed the *neural network for graphs* (NN4G) model, which focused on a *feedforward* rather than recurrent paradigm (Micheli, 2009).

Computational chemistry It is also very important to note an independent and concurrent line of development for GNNs: one that was entirely driven by the needs of computational chemistry, where molecules are most naturally expressed as graphs of atoms (nodes) connected by chemical bonds (edges). This invited computational techniques for molecular property prediction that operate directly over such a graph structure, which had become present in machine learning in the 1990s: this includes the ChemNet model of Kireev (1995) and the work of Baskin et al. (1997). Strikingly, the "molecular graph networks" of Merkwirth and Lengauer (2005) explicitly proposed many of the elements commonly found in contemporary GNNs—such as edge type-conditioned weights or global pooling—as early as 2005. The chemical motivation continued to drive GNN development into the 2010s, with two significant GNN advancements centered around improving molecular fingerprinting (Duvenaud et al., 2015) and predicting quantum-chemical properties (Gilmer et al., 2017) from small molecules. At the time of writing this text, molecular property prediction is one of the most successful applications of GNNs, with impactful results in virtual screening of new antibiotic drugs (Stokes et al., 2020).

Node embeddings Some of the earliest success stories of deep learning on graphs involve learning representations of nodes in an unsupervised fashion, based on the graph structure. Given their structural inspiration, this direction also provides one of the most direct links between graph representation learning and network science communities. The key early

approaches in this space relied on *random walk*-based embeddings: learning node representations in a way that brings them closer together if the nodes co-occur in a short random walk. Representative methods in this space include DeepWalk (Perozzi et al., 2014), node2vec (Grover and Leskovec, 2016) and LINE (Tang et al., 2015), which are all purely self-supervised. Planetoid (Yang et al., 2016) was the first in this space to incorporate supervision label information, when it is available.

Recently, a theoretical framework was developed by Srinivasan and Ribeiro (2019) in which the equivalence of structural and positional representations was demonstrated. Additionally, Qiu et al. (2018) have demonstrated that all random-walk based embedding techniques are equivalent to an appropriately-posed matrix factorisation task.

Unifying random walk objectives with GNN encoders was attempted on several occasions, with representative approaches including Variational Graph Autoencoder (VGAE, Kipf and Welling (2016b)), embedding propagation (García-Durán and Niepert, 2017), and unsupervised variants of GraphSAGE (Hamilton et al., 2017). However, this was met with mixed results, and it was shortly discovered that pushing neighbouring node representations together is already a key part of GNNs' inductive bias. Indeed, it was shown that an *untrained* GNN was already showing performance that is competitive with DeepWalk, in settings where node features are available (Veličković et al., 2019; Wu et al., 2019). This launched a direction that moves away from combining random walk objectives with GNNs and shifting towards *contrastive* approaches inspired by mutual information maximisation and aligning to successful methods in the image domain. Prominent examples of this direction include Deep Graph Informax (DGI, Veličković et al. (2019)), GRACE (Zhu et al., 2020), BERT-like objectives (Hu et al., 2020) and BGRL (Thakoor et al., 2021).

Probabilistic graphical models Graph neural networks have also, concurrently, resurged through embedding the computations of *probabilistic graphical models* (PGMs, Wainwright and Jordan (2008)). PGMs are a powerful tool for processing graphical data, and their utility arises from their probabilistic perspective on the graph's edges: namely, the nodes are treated as *random variables*, while the graph structure encodes *conditional independence* assumptions, allowing for significantly simplifying the calculation and sampling from the joint distribution. Indeed, many algorithms for (exactly or approximately) supporting learning and inference on PGMs rely on forms of passing messages over their edges (Pearl, 2014), with examples including variational mean-field inference and loopy belief propagation (Yedidia et al., 2001; Murphy et al., 2013).

This connection between PGMs and message passing was subsequently

developed into GNN architectures, with early theoretical links established by the authors of structure2vec (Dai et al., 2016). Namely, by posing a graph representation learning setting as a Markov random field (of nodes corresponding to input features and latent representations), the authors directly align the computation of both mean-field inference and loopy belief propagation to a model not unlike the GNNs commonly in use today.

The key "trick" which allowed for relating the latent representations of a GNN to probability distributions maintained by a PGM was the usage of *Hilbert-space embeddings* of distributions (Smola et al., 2007). Given ϕ, an appropriately chosen embedding function for features $\mathbf{x}$, it is possible to embed their probability distribution $p(\mathbf{x})$ as the *expected* embedding $\mathbb{E}_{\mathbf{x}\sim p(\mathbf{x})}\phi(\mathbf{x})$. Such a correspondence allows us to perform GNN-like computations, knowing that the representations computed by the GNN will always correspond to an embedding of *some* probability distribution over the node features.

The structure2vec model itself is, ultimately, a GNN architecture which easily sits within our framework, but its setup has inspired a series of GNN architectures which more directly incorporate computations found in PGMs. Emerging examples have successfully combined GNNs with conditional random fields (Gao et al., 2019; Spalević et al., 2020), relational Markov networks (Qu et al., 2019) and Markov logic networks (Zhang et al., 2020).

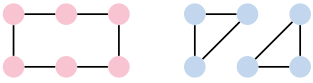
The Weisfeiler-Lehman formalism The resurgence of graph neural networks was followed closely by a drive to understand their fundamental limitations, especially in terms of expressive power. While it was becoming evident that GNNs are a strong modelling tool of graph-structured data, it was also clear that they wouldn't be able to solve *any* task specified on a graph perfectly. A canonical illustrative example of this is deciding *graph isomorphism*: is our GNN able to attach different representations to two given non-isomorphic graphs? This is a useful framework for two reasons. If the GNN is unable to do this, then it will be hopeless on any task requiring the discrimination of these two graphs. Further, it is currently not known if deciding graph isomorphism is in P, the complexity class in which all GNN computations typically reside.

Due to their permutation invariance, GNNs will attach identical representations to two isomorphic graphs, so this case is trivially solved.

The best currently known algorithm for deciding graph isomorphism is due to Babai and Luks (1983), though a recent (not fully reviewed) proposal by Babai (2016) implies a quasi-polynomial time solution.

The key framework which binds GNNs to graph isomorphism is the *Weisfeiler-Lehman* (WL) graph isomorphism test (Weisfeiler and Leman, 1968). This test generates a graph representation by iteratively passing node features

along the edges of the graph, then *randomly hashing* their sums across neighbourhoods. Connections to *randomly-initialised* convolutional GNNs are apparent, and have been observed early on: for example, within the GCN model of Kipf and Welling (2016a). Aside from this connection, the WL iteration was previously introduced in the domain of *graph kernels* by Shervashidze et al. (2011), and it still presents a strong baseline for unsupervised learning of whole-graph representations.



One simple example: the WL test cannot distinguish a *6-cycle* from *two triangles*.

While the WL test is conceptually simple, and there are many simple examples of non-isomorphic graphs it cannot distinguish, its expressive power is ultimately strongly tied to GNNs. Analyses by Morris et al. (2019) and Xu et al. (2018) have both reached a striking conclusion: *any* GNN conforming to one of the three flavours we outlined in Section 5.3 cannot be more powerful than the WL test!

Popular aggregators such as maximisation and averaging fall short in this regard, because they would not be able to distinguish e.g. the neighbour multisets $\{\!\{\mathbf{a}, \mathbf{b}\}\!\}$ and $\{\!\{\mathbf{a}, \mathbf{a}, \mathbf{b}, \mathbf{b}\}\!\}$.

In order to exactly reach this level of representational power, certain constraints must exist on the GNN update rule. Xu et al. (2018) have shown that, in the discrete-feature domain, the aggregation function the GNN uses must be *injective*, with *summation* being a key representative. Based on the outcome of their analysis, Xu et al. (2018) propose the Graph Isomorphism Network (GIN), which is a simple but powerful example of a maximally-expressive GNN under this framework. It is also expressible under the convolutional GNN flavour we propose.

One example of such aggregators are the *moments* of the multiset of neighbours.

Lastly, it is worth noting that these findings do not generalise to *continuous* node feature spaces. In fact, using the Borsuk-Ulam theorem (Borsuk, 1933), Corso et al. (2020) have demonstrated that, assuming real-valued node features, obtaining injective aggregation functions requires *multiple* aggregators (specifically, equal to the *degree* of the receiver node). Their findings have driven the Principal Neighbourhood Aggregation (PNA) architecture, which proposes a multiple-aggregator GNN that is empirically powerful and stable.

Higher-order methods The findings of the previous paragraphs do not contradict the practical utility of GNNs. Indeed, in many real-world applications the input features are sufficiently *rich* to support useful discriminative computations over the graph structure, despite of the above limitations.

Which, in contrast, almost always consider *featureless* or *categorically-featured* graphs.

However, one key corollary is that GNNs are relatively quite weak at detecting some rudimentary *structures* within a graph. Guided by the specific

limitations or failure cases of the WL test, several works have provided *stronger* variants of GNNs that are *provably* more powerful than the WL test, and hence likely to be useful on tasks that require such structural detection.

One prominent example is computational chemistry, wherein a molecule's chemical function can be strongly influenced by the presence of aromatic *rings* in its molecular graph.

Perhaps the most direct place to hunt for more expressive GNNs is the WL test itself. Indeed, the strength of the original WL test can be enhanced by considering a *hierarchy* of WL tests, such that k-WL tests attach representations to k-*tuples* of nodes (Morris et al., 2017). The k-WL test has been directly translated into a *higher-order* k-GNN architecture by Morris et al. (2019), which is provably more powerful than the GNN flavours we considered before. However, its requirement to maintain tuple representations implies that, in practice, it is hard to scale beyond $k = 3$.

There have been efforts, such as the δ-k-LGNN (Morris et al., 2020), to sparsify the computation of the k-GNN.

Concurrently, Maron et al. (2018, 2019) have studied the characterisation of invariant and equivariant graph networks over k-tuples of nodes. Besides demonstrating the surprising result of *any* invariant or equivariant graph network being expressible as a linear combination of a finite number of generators—the amount of which only depends on k—the authors showed that the expressive power of such layers is equivalent to the k-WL test, and proposed an empirically scalable variant which is provably 3-WL powerful.

Besides generalising the domain over which representations are computed, significant effort had also went into analysing specific failure cases of 1-WL and augmenting GNN *inputs* to help them distinguish such cases. One common example is attaching *identifying features* to the nodes, which can help detecting structure. Proposals to do this include *one-hot* representations (Murphy et al., 2019), as well as purely *random* features (Sato et al., 2020).

For example, if a node sees its own identifier k hops away, it is a direct indicator that it is within a k-cycle.

More broadly, there have been many efforts to incorporate *structural* information within the message passing process, either by modulating the message function or the graph that the computations are carried over. Several interesting lines of work here involve sampling *anchor node sets* (You et al., 2019), aggregating based on *Laplacian eigenvectors* (Stachenfeld et al., 2020; Beaini et al., 2020; Dwivedi and Bresson, 2020), or performing *topological data analysis*, either for positional embeddings (Bouritsas et al., 2020) or driving message passing (Bodnar et al., 2021).

In the computational chemistry domain, it is often assumed that molecular function is driven by substructures (the *functional groups*), which have directly inspired the modelling of molecules at a *motif* level. For references, consider Jin et al. (2018, 2020); Fey et al. (2020).

Signal processing and Harmonic analysis Since the early successes of Convolutional Neural Networks, researchers have resorted to tools from harmonic analysis, image processing, and computational neuroscience trying to

provide a theoretical framework that explains their efficiency. M-theory is a framework inspired by the visual cortex, pioneered by Tomaso Poggio and collaborators (Riesenhuber and Poggio, 1999; Serre et al., 2007), based on the notion of templates that can be manipulated under certain symmetry groups. Another notable model arising from computational neuroscience were *steerable pyramids*, a form of multiscale wavelet decompositions with favorable properties against certain input transformations, developed by Simoncelli and Freeman (1995). They were a central element in early generative models for textures (Portilla and Simoncelli, 2000), which were subsequently improved by replacing steerable wavelet features with deep CNN features Gatys et al. (2015). Finally, Scattering transforms, introduced by Stéphane Mallat (2012) and developed by Bruna and Mallat (2013), provided a framework to understand CNNs by replacing trainable filters with multiscale wavelet decompositions, also showcasing the deformation stability and the role of depth in the architecture.

Signal Processing on Graph and Meshes Another important class of graph neural networks, often referred to as *spectral*, has emerged from the work of one of the authors of this text (Bruna et al., 2013), using the notion of the *Graph Fourier transform*. The roots of this construction are in the signal processing and computational harmonic analysis communities, where dealing with non-Euclidean signals has become prominent in the late 2000s and early 2010s. Influential papers from the groups of Pierre Vandergheynst (Shuman et al., 2013) and José Moura (Sandryhaila and Moura, 2013) popularised the notion of "Graph Signal Processing" (GSP) and the generalisation of Fourier transforms based on the eigenvectors of graph adjacency and Laplacian matrices. The graph convolutional neural networks relying on spectral filters by Defferrard et al. (2016) and Kipf and Welling (2016a) are among the most cited in the field and can likely be credited) as ones reigniting the interest in machine learning on graphs in recent years.

It is worth noting that, in the field of computer graphics and geometry processing, non-Euclidean harmonic analysis predates Graph Signal Processing by at least a decade. We can trace spectral filters on manifolds and meshes to the works of Taubin et al. (1996). These methods became mainstream in the 2000s following the influential papers of Karni and Gotsman (2000) on spectral geometry compression and of Lévy (2006) on using the Laplacian eigenvectors as a non-Euclidean Fourier basis. Spectral methods have been used for a range of applications, most prominent of which is the construction

Learnable shape descriptors similar to spectral graph CNNs were proposed by Roee Litman and Alex Bronstein (2013), the latter being a twin brother of the author of this text.

of shape descriptors (Sun et al., 2009) and functional maps (Ovsjanikov et al., 2012); these methods are still broadly used in computer graphics at the time of writing.

Computer Graphics and Geometry Processing Models for shape analysis based on intrinsic metric invariants were introduced by various authors in the field of computer graphics and geometry processing (Elad and Kimmel, 2003; Mémoli and Sapiro, 2005; Bronstein et al., 2006), and are discussed in depth by one of the authors in his earlier book (Bronstein et al., 2008). The notions of intrinsic symmetries were also explored in the same field Raviv et al. (2007); Ovsjanikov et al. (2008). The first architecture for deep learning on meshes, Geodesic CNNs, was developed in the team of one of the authors of the text (Masci et al., 2015). This model used local filters with shared weights, applied to geodesic radial patches. It was a particular setting of gauge-equivariant CNNs developed later by another author of the text (Cohen et al., 2019). A generalisation of Geodesic CNNs with learnable aggregation operations, MoNet, proposed by Federico Monti et al. (2017) from the same team, used an attention-like mechanism over the local structural features of the mesh, that was demonstrated to work on general graphs as well. The graph attention network (GAT), which technically speaking can be considered a particular instance of MoNet, was introduced by another author of this text (Veličković et al., 2018). GATs generalise MoNet's attention mechanism to also incorporate node feature information, breaking away from the purely structure-derived relevance of prior work. It is one of the most popular GNN architectures currently in use.

In the context of computer graphics, it is also worthwhile to mention that the idea of learning on sets (Zaheer et al., 2017) was concurrently developed in the group of Leo Guibas at Stanford under the name PointNet (Qi et al., 2017) for the analysis of 3D point clouds. This architecture has lead to multiple follow-up works, including one by an author of this text called Dynamic Graph CNN (DGCNN, Wang et al. (2019b)). DGCNN used a nearest-neighbour graph to capture the local structure of the point cloud to allow exchange of information across the nodes; the key characteristic of this architecture was that the graph was constructed on-the-fly and updated between the layers of the neural network in relation to the downstream task. This latter property made DGCNN one of the first incarnations of 'latent graph learning', which in its turn has had significant follow up. Extensions to DGCNN's k-nearest neighbour graph proposal include more explicit control

over these graphs' edges, either through bilevel optimisation (Franceschi et al., 2019), reinforcement learning (Kazi et al., 2020) or direct supervision (Veličković et al., 2020). Independently, a variational direction (which probabilistically samples edges from a computed *posterior* distribution) has emerged through the NRI model (Kipf et al., 2018). While it still relies on quadratic computation in the number of nodes, it allows for explicitly encoding uncertainty about the chosen edges.

Another very popular direction in learning on graphs without a provided graph relies on performing GNN-style computations over a *complete* graph, letting the network infer its own way to exploit the connectivity. The need for this arisen particularly in natural language processing, where various words in a sentence interact in highly nontrivial and non-sequential ways. Operating over a complete graph of words brought about the first incarnation of the Transformer model (Vaswani et al., 2017), which de-throned both recurrent and convolutional models as state-of-the-art in neural machine translation, and kicked off an avalanche of related work, transcending the boundaries between NLP and other fields. Fully-connected GNN computation has also concurrently emerged on simulation (Battaglia et al., 2016), reasoning (Santoro et al., 2017), and multi-agent (Hoshen, 2017) applications, and still represents a popular choice when the number of nodes is reasonably small.

Algorithmic reasoning For most of the discussion we posed in this section, we have given examples of *spatially* induced geometries, which in turn shape the underlying domain, and its invariances and symmetries. However, plentiful examples of invariances and symmetries also arise in a *computational* setting. One critical difference to many common settings of Geometric Deep Learning is that links no longer need to encode for any kind of similarity, proximity, or types of relations—they merely specify the "recipe" for the dataflow between data points they connect.

Instead, the computations of the neural network mimic the reasoning process of an *algorithm* (Cormen et al., 2009), with additional invariances induced by the algorithm's control flow and intermediate results. In the space of algorithms the assumed input invariants are often referred to as *preconditions*, while the invariants preserved by the algorithm are known as *postconditions*.

For example, one invariant of the Bellman-Ford pathfinding algorithm (Bellman, 1958) is that, after k steps, it will always compute the shortest paths to the source node that use no more than k edges.

Eponymously, the research direction of *algorithmic reasoning* (Cappart et al., 2021, Section 3.3.) seeks to produce neural network architectures that ap-

propriately preserve algorithmic invariants. The area has investigated the construction of general-purpose neural computers, e.g., the *neural Turing machine* (Graves et al., 2014) and the *differentiable neural computer* (Graves et al., 2016). While such architectures have all the hallmarks of general computation, they introduced several components at once, making them often challenging to optimise, and in practice, they are almost always outperformed by simple relational reasoners, such as the ones proposed by Santoro et al. (2017, 2018).

As modelling complex postconditions is challenging, plentiful work on inductive biases for learning to execute (Zaremba and Sutskever, 2014) has focused on primitive algorithms (e.g. simple arithmetic). Prominent examples in this space include the *neural GPU* (Kaiser and Sutskever, 2015), *neural RAM* (Kurach et al., 2015), *neural programmer-interpreters* (Reed and De Freitas, 2015), *neural arithmetic-logic units* (Trask et al., 2018; Madsen and Johansen, 2020) and *neural execution engines* (Yan et al., 2020).

Emulating combinatorial algorithms of *superlinear* complexity was made possible with the rapid development of GNN architectures. The *algorithmic alignment* framework pioneered by Xu et al. (2019) demonstrated, theoretically, that GNNs *align* with dynamic programming (Bellman, 1966), which is a language in which most algorithms can be expressed. It was concurrently empirically shown, by one of the authors of this text, that it is possible to design and train GNNs that align with algorithmic invariants in practice (Veličković et al., 2019). Onwards, alignment was achieved with *iterative algorithms* (Tang et al., 2020), *linearithmic algorithms* (Freivalds et al., 2019), *data structures* (Veličković et al., 2020) and *persistent memory* (Strathmann et al., 2021). Such models have also seen practical use in *implicit planners* (Deac et al., 2020), breaking into the space of *reinforcement learning* algorithms.

Concurrently, significant progress has been made on using GNNs for *physics simulations* (Sanchez-Gonzalez et al., 2020; Pfaff et al., 2020). This direction yielded much of the same recommendations for the design of generalising GNNs. Such a correspondence is to be expected: given that algorithms can be phrased as discrete-time simulations, and simulations are typically implemented as step-wise algorithms, both directions will need to preserve similar kinds of invariants.

Tightly bound with the study of algorithmic reasoning are measures of *extrapolation*. This is a notorious pain-point for neural networks, given that most of their success stories are obtained when generalising *in-distribution*;

i.e. when the patterns found in the training data properly anticipate the ones found in the test data. However, algorithmic invariants must be preserved irrespective of, e.g., the size or generative distribution of the input, meaning that the training set will likely not cover any possible scenario encountered in practice. Xu et al. (2020b) have proposed a geometric argument for what is required of an extrapolating GNN backed by rectifier activations: its components and featurisation would need to be designed so as to make its constituent modules (e.g. message function) learn only *linear* target functions. Bevilacqua et al. (2021) propose observing extrapolation under the lens of *causal reasoning*, yielding *environment-invariant* representations of graphs.

Geometric Deep Learning Our final historical remarks regard the very name of this text. The term 'Geometric Deep Learning' was first introduced by one of the authors of this text in his ERC grant in 2015 and popularised in the eponymous IEEE Signal Processing Magazine paper (Bronstein et al., 2017). This paper proclaimed, albeit "with some caution", the signs of "a new field being born." Given the recent popularity of graph neural networks, the increasing use of ideas of invariance and equivariance in a broad range of machine learning applications, and the very fact of us writing this text, it is probably right to consider this prophecy at least partially fulfilled. The name "4G: Grids, Graphs, Groups, and Gauges" was coined by Max Welling for the ELLIS Program on Geometric Deep Learning, co-directed by two authors of the text. Admittedly, the last 'G' is somewhat of a stretch, since the underlying structures are manifolds and bundles rather than gauges. For this text, we added another 'G', Geodesics, in reference to metric invariants and intrinsic symmetries of manifolds.

Acknowledgements

This text represents a humble attempt to summarise and synthesise decades of existing knowledge in deep learning architectures, through the geometric lens of invariance and symmetry. We hope that our perspective will make it easier both for newcomers and practitioners to navigate the field, and for researchers to synthesise novel architectures, as instances of our blueprint. In a way, we hope to have presented *"all you need to build the architectures that are all you need"*—a play on words inspired by Vaswani et al. (2017).

The bulk of the text was written during late 2020 and early 2021. As it often happens, we had thousands of doubts whether the whole picture makes sense, and used opportunities provided by our colleagues to help us break our "stage fright" and present early versions of our work, which saw the light of day in Petar's talk at Cambridge (courtesy of Pietro Liò) and Michael's talks at Oxford (courtesy of Xiaowen Dong) and Imperial College (hosted by Michael Huth and Daniel Rueckert). Petar was also able to present our work at Friedrich-Alexander-Universität Erlangen-Nürnberg—the birthplace of the Erlangen Program!—owing to a kind invitation from Andreas Maier. The feedback we received for these talks was enormously invaluable to keeping our spirits high, as well as polishing the work further. Last, but certainly not least, we thank the organising committee of ICLR 2021, where our work will be featured in a keynote talk, delivered by Michael.

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