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# Automated Deep Learning: Neural Architecture Search Is Not the End

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# Foundations and Trends® in Machine Learning

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# Automated Deep Learning: Neural Architecture Search Is Not the End

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## ABSTRACT

Deep learning (DL) has proven to be a highly effective approach for developing models in diverse contexts, including visual perception, speech recognition, and machine translation. However, the end-to-end process for applying DL is not trivial. It requires grappling with problem formulation and context understanding, data engineering, model development, deployment, continuous monitoring and maintenance, and so on. Moreover, each of these steps typically relies heavily on humans, in terms of both knowledge and interactions, which impedes the further advancement and democratization of DL. Consequently, in response to these issues, a new field has emerged over the last few years: automated deep learning (AutoDL). This endeavor seeks to minimize the need for human involvement and is best known for its achievements in neural architecture search (NAS), a topic that has been the focus of several surveys. That stated,

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NAS is not the be-all and end-all of AutoDL. Accordingly, this review adopts an overarching perspective, examining research efforts into automation across the entirety of an archetypal DL workflow. In so doing, this work also proposes a comprehensive set of ten criteria by which to assess existing work in both individual publications and broader research areas. These criteria are: novelty, solution quality, efficiency, stability, interpretability, reproducibility, engineering quality, scalability, generalizability, and eco-friendliness. Thus, ultimately, this review provides an evaluative overview of AutoDL in the early 2020s, identifying where future opportunities for progress may exist.

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**Keywords:** Automated deep learning (AutoDL); neural architecture search (NAS); hyperparameter optimization (HPO); automated data engineering; hardware search; automated deployment; life-long learning; persistent learning; adaptation; automated machine learning (AutoML); autonomous machine learning (AutonoML); deep neural networks; deep learning.

# 1

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## Introduction

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In the quest for artificial intelligence (AI), history may judge the early 2010s as a mental reset, stimulating a new era of research and development with unrivaled intensity. Within those reformative years, the field of machine learning (ML) witnessed a shifting of priorities and approaches. Two threads of aspiration stand out:

- Deep Learning (DL) – The idea that multi-layered artificial-neuron networks are central to pushing the capabilities of ML.
- Automated Machine Learning (AutoML) – The idea that no part of an ML workflow should necessarily depend on human involvement.

It was inevitable that these two ideologies would eventually converge, fusing into the novel subject of automated deep learning (AutoDL).

Admittedly, while AutoDL is a “hot topic” in 2021, the foundations underlying this surge of activity stretch back for decades. The notion of ML itself (Michie *et al.*, 1994) was established in the 1950s, aiming to tune mathematical models of desirable functions via automated data-driven algorithms. In time, by the turn of the 21st century, numerous ML models and algorithms would be in practical use, with

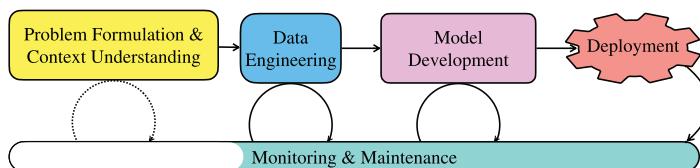
support vector machines and other kernel methods proving particularly popular (Hofmann *et al.*, 2008). However, the concept of a neuron, intrinsically linked to human intelligence, always seemed an obvious basis for ML. Depicted computationally as early as the 1940s (McCulloch and Pitts, 1943), their representational power in multi-layered arrangements was evident by the late 1960s, exemplified by the proto-DL “group method of data handling” (GMDH) (Ivakhnenko, 1971). Since then, with stutters around AI winters, numerous types of neural layers and architectural variants have been proposed and adopted. These include recurrent structures (Hopfield, 1982; Little, 1974), convolutional and downsample layers (Fukushima and Miyake, 1982), auto-encoder hierarchies (Ballard, 1987), memory mechanisms (Pollack, 1989), and gating structures (Hochreiter and Schmidhuber, 1997).

As a result, the historical successes of artificial neural networks (ANNs) are undeniably many, encompassing handwriting recognition (LeCun *et al.*, 1989), time series prediction (Weigend and Gershenfeld, 1993), video retrieval (Ji *et al.*, 2012; Yang *et al.*, 2009), mitosis detection (Cireşan *et al.*, 2013), and so on. Yet the advantages of deep neural networks (DNNs), including their status as universal approximators (Hornik *et al.*, 1989), are countered by the unwieldy nature of their complexity. For instance, while backpropagation was established as reverse automatic differentiation in the 1970s (Linnainmaa, 1970), this DNN training technique did not become generally feasible until relatively recently. Thus, the rising dominance of DL in the 2010s (LeCun *et al.*, 2015; Schmidhuber, 2015) is as much an outcome of big data infrastructure and hardware acceleration, specifically graphical processing units (GPUs), as it is the result of any one theoretical advance.

In contrast, the evolution of AutoML is harder to pin down, primarily because the scope of automating higher-level ML mechanisms can be made extremely broad. The extended history of this topic is grappled with elsewhere (Kedziora *et al.*, 2020). Nonetheless, the mainstream interpretation of AutoML – and even the abbreviation itself – has been forged on the back of advances in ML model/algorithm selection and the optimization of their user-defined hyperparameters. Accordingly, if the success of a DNN in the 2012 ImageNet competition (Krizhevsky *et al.*, 2012) heralds the modern DL era, then the release of Auto-WEKA in

2013 (Thornton *et al.*, 2013) marks the start of the modern AutoML era. Within several years, by late 2016, these threads would start to entwine within the sub-field of neural architecture search (NAS) (Baker *et al.*, 2017; Zoph and Le, 2017). This was not the first time that AutoML techniques had been applied to neural networks, but it was the moment that the broader data science community took notice. It was also opportune; the website Papers-With-Code (Facebook AI Research, n.d.) highlights that, while the number of DL publications has skyrocketed since 2012, year-by-year performance improvements on many benchmark datasets have diminished, i.e., those related to vision, text, audio, and speech. There is a sense that, as state-of-the-art (SoTA) DL models have become highly sophisticated, a reliance on human design is locking out broader engagement behind steep learning curves, while also hindering further metric progress. Automation through NAS is a vital step in enabling a broader community to push these technical limits.

Importantly, while NAS launched the modern AutoDL story, it does not encompass it. Model selection, i.e., the design of a neural network, is but one stage of a DL workflow. As illustrated in Figure 1.1, there are many other subtasks involved in ML/DL, such as defining a problem of interest, collecting and organizing data, generating features, deploying and adapting trained models. This workflow may often be sequential in research and development, but real-world applications are much more agile and will typically reiterate through earlier operations and, in the case of large-scale systems, these processes may even be asynchronous. In effect, AI based on DL cannot reach its full potential



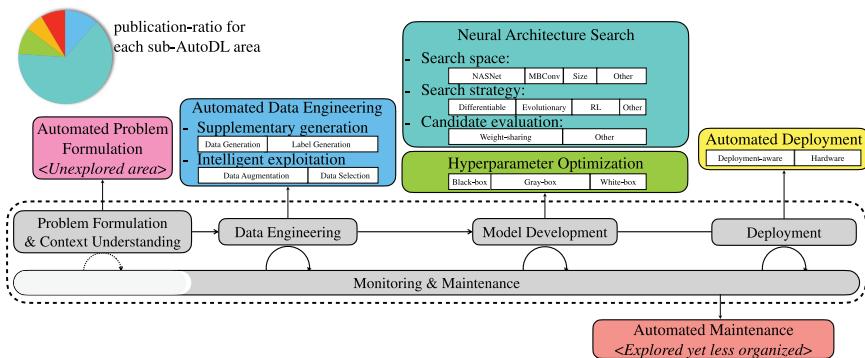
**Figure 1.1:** Schematic of an end-to-end DL workflow, i.e., the processes involved in applying DL to a problem. Traditionally, human decisions are required for every part of this workflow, such as analyzing a problem context, defining an ML task, designing a model, manually tuning hyperparameters, selecting training strategy.

without considering the entire life cycle of a solution, from its design to the maintenance phase.

We now bring attention to a previous review (Kedziora *et al.*, 2020), which surveyed efforts to automate all aspects of this workflow in the general context of ML, with additional focus on how the resulting mechanisms may be integrated into a single architecture. The review touched on NAS and other elements of DL, but it could not cover the full extent of work in the AutoDL sphere. It did not need to; at a high level, working with DNNs fits smoothly into the conceptual framework of both AutoML and its extension, autonomous machine learning (AutonoML). However, on a practical level, the complexity of DNNs throws up many challenges that have arguably constrained the breadth of developments in AutoDL as compared to standard AutoML. Instead, what is remarkable is the *depth* of research in AutoDL, with numerous innovations brought about by attempts to surmount these obstacles, all with the aim of making the automation of DL feasible. Certainly, it would be remiss to trivialize AutoDL as just a subset of AutoML. Likewise, critically evaluating the limitations of present-day AutoDL is just as worthwhile as highlighting its accomplishments. For instance, the field of DL is sometimes criticized for a tunnel-vision focus on model-performance metrics within a limited set of benchmarks, an attitude which, while valid, risks missing the broader perspective on all that AutoDL may become (Dong *et al.*, 2021a; Gencoglu *et al.*, 2019). In essence, there is a need to consider several questions more thoroughly:

- As we enter the 2020s, what is the current research landscape of DL?
- What makes a “good” DL model?
- How can automated systems best pursue and support this model performance?
- Is the field of AutoDL even advanced enough for such a meta-analysis?

This work is an extension of the broadly scoped AutonoML review (Kedziora *et al.*, 2020) with an in-depth focus on the newly



**Figure 1.2:** (Color online) breakdown schematic for research activity in AutoDL, with surveyed publications attributed to different phases of a DL workflow and then further subcategorized. The pie chart denotes the ratio of publications across all workflow phases, while the white stacked bars denote ratios within each subcategory. All statistics are derived from the Awesome-AutoDL project, at: <https://github.com/D-X-Y/Awesome-AutoDL>.

popularized topic of AutoDL. While there are many surveys in this sphere<sup>1</sup> (Elsken *et al.*, 2019; Feurer and Hutter, 2019; Ren *et al.*, 2021; Wistuba *et al.*, 2019; Yu and Zhu, 2020), most focus on deep analysis within one or two sub-domains of AutoDL. In contrast, we examine the entire spectrum of the DL workflow, as of 2021, actively identifying areas that have not yet been fully explored or where automation research may still be in its infancy. We first provide an overview of AutoDL in Section 2, introducing several fundamental concepts. Then, partitioning major AutoDL research into sections inspired by a DL workflow, as per Figure 1.2, we explore automation for: task management (Section 3), data preparation (Section 4), neural architecture design (Section 5), hyperparameter selection (Section 6), model deployment (Section 7), and online maintenance (Section 8).

Crucially, a major motivation for this review is a reaction to the sheer quantity of publications in the space of AutoDL; we aim to provide summary assessments of surveyed AutoDL algorithms/research in terms of ten carefully designed criteria, not just accuracy alone. These

<sup>1</sup>One of the authors maintains a publicly accessible curated list of AutoDL resources at: <https://github.com/D-X-Y/Awesome-AutoDL>.

are introduced in Section 2.4 and form an evaluative framework for overviews within every aforementioned section, as well as, in Section 9, a final critical discussion around the entire field of AutoDL.

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