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AutonoML: Towards an Integrated Framework for Autonomous Machine Learning

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AutonoML: Towards an Integrated Framework for Autonomous Machine Learning

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ABSTRACT

Over the last decade, the long-running endeavour to automate high-level processes in machine learning (ML) has risen to mainstream prominence, stimulated by advances in optimisation techniques and their impact on selecting ML models/algorithms. Central to this drive is the appeal of engineering a computational system that both discovers and deploys high-performance solutions to arbitrary ML problems with minimal human interaction. Beyond this, an even loftier goal is the pursuit of autonomy, which describes the capability of the system to independently adjust an ML solution over a lifetime of changing contexts. However, these ambitions are unlikely to be achieved in a robust manner without the broader synthesis of various mechanisms and theoretical frameworks, which, at the present time, remain scattered across numerous research threads. Accordingly, this review seeks to motivate a more expansive perspective

on what constitutes an automated/autonomous ML system, alongside consideration of how best to consolidate those elements. In doing so, we survey developments in the following research areas: hyperparameter optimisation, multi-component models, neural architecture search, automated feature engineering, meta-learning, multi-level ensembling, dynamic adaptation, multi-objective evaluation, resource constraints, flexible user involvement, and the principles of generalisation. We also develop a conceptual framework throughout the review, augmented by each topic, to illustrate one possible way of fusing high-level mechanisms into an autonomous ML system. Ultimately, we conclude that the notion of architectural integration deserves more discussion, without which the field of automated ML risks stifling both its technical advantages and general uptake.

1

Introduction

The field of data science is primarily concerned with the process of extracting information from data, often by way of fitting a mathematical model. Data science, as an umbrella term for techniques drawn from various disciplines, is agnostic as to who or what is driving that extraction. Indeed, while much effort has been dedicated to codifying effective workflows for data scientists (Fayyad *et al.*, 1996), e.g. the Cross-Industry Standard Process for Data Mining (CRISP-DM) (Chapman *et al.*, 2000) and others (Kurgan and Musilek, 2006; Studer *et al.*, 2021), there is no inherent restriction that forces any phase of the process to be manually applied.

Certainly, in the modern era, one element of data mining and analysis is almost ubiquitously automated: model training. At one point in time, this was considered a novel advance, with computers only just becoming capable of running model-updating algorithms, as depicted in Figure 1.1, without human intervention. In fact, this form of automation was considered such a paradigm shift that it birthed the term ‘machine learning’ (ML) in the 1950s (Samuel, 1959), provoked debate on its “moral and technical consequences” (Wiener, 1960; Samuel, 1960), and merged into the evolution of modern data analysis (Tukey,

1962). Advances since then, both fundamental and technological, have all but cemented computational dominance for model training.

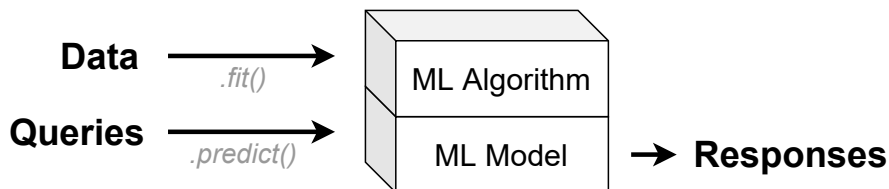


Figure 1.1: A simple representation of a machine learning (ML) model, which takes in user queries and outputs responses. The ML model is tuned by an ML algorithm, which processes training data.

Now, more than 60 years beyond the dawn of ML, associated techniques and technologies have diffused through society at large. While advances in graphics processing units (GPUs) and big data architectures are credited with popularising deep neural networks (DNNs), abundant black-box implementations of the backpropagation method have also played their part. In effect, the need for human expertise to develop complex inferential models has been lessened, and the last decade has consequently witnessed data science moving towards democratisation (Bond *et al.*, 2019). The 2012 journal article that is frequently credited with kicking off the DNN era sums it up well: “What many in the vision research community failed to appreciate was that methods that require careful hand-engineering by a programmer who understands the domain do not scale as well as methods that replace the programmer with a powerful general-purpose learning procedure.” (Krizhevsky *et al.*, 2012)

Despite all this, common practice has not yet seen widespread mechanisation along the rest of the data science chain (Vega *et al.*, 2019). Granted, given a specific choice of model, it is routine to train, validate and deploy the model on clean and informative datasets with ‘fit’ and ‘predict’ functionality, depicted in Figure 1.1, that is provided by numerous coding packages. However, even within the model-development phase, the typical data scientist still has to select a model, an evaluation metric and a training/validation strategy, all subject to human bias. Once the entire ML workflow is considered, shown at high level in

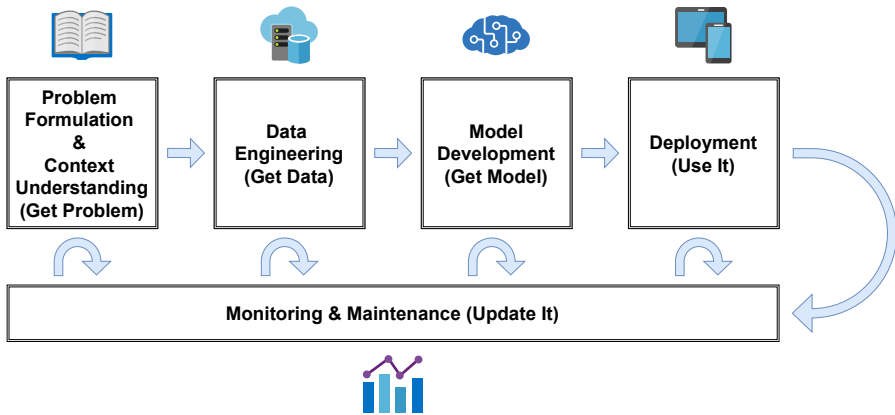


Figure 1.2: Schematic of the workflow involved in designing, constructing, deploying and maintaining an ML model. Crucially, monitoring and maintenance are required to enable continuous learning, a prerequisite for autonomous machine learning (AutoML).

Figure 1.2, it becomes even more clear just how much an ML application relies on manual operations, which is not ideal. The data-engineering phase, for instance, is a notorious time sink for human involvement (Cios and Kurgan, 2005; Kurgan and Musilek, 2006).

The field of ‘automated machine learning’ (AutoML) (Hutter *et al.*, 2019; Yao *et al.*, 2018; He *et al.*, 2019; Zöllner and Huber, 2021; Balaji and Allen, 2018; Truong *et al.*, 2019) has firmly established itself in recent years as a response to this; AutoML endeavours to continue mechanising the workflow of ML-based operations. It is motivated by the idea that reducing dependencies on human effort and expertise will, as a non-exhaustive list,

- make ML and its benefits more accessible to the general public,
- improve the efficiency and speed of finding ML solutions,
- improve the quality and consistency of ML solutions,
- enforce a systematic application of sound and robust ML methodologies,
- enable quick deployment and reuse of ML methodologies,

- compartmentalise complexity to reduce the potential for human error, and
- divert human resources to more productive roles.

In fairness, the field as a whole must also grapple with the risks of automation, including,

- increased obscuration of ML technical debt (Sculley *et al.*, 2015),
- inappropriate or unethical usage as a result of ML illiteracy (Bond *et al.*, 2019),
- interpretability issues in high-stakes contexts (Rudin, 2019), and
- adverse socio-economic impacts such as job displacement (Wang and Siau, 2019).

These are complex topics that are deserving of their own extensive discussions.

In this review, we focus primarily on the technical aspects of AutoML. Specifically, we motivate and discuss synthesising major threads of existing AutoML research into a general integrated framework. Unlike other published reviews, we also broaden the scope to capture adjacent research that has been, to date, barely or not at all associated with the AutoML label, particularly in recent scientific literature. In effect, the aim of this review is to help inspire the evolution of AutoML towards ‘autonomous machine learning’ (AutonoML), where architectures are able to independently design, construct, deploy, and maintain ML models to solve specific problems, ideally limiting human involvement to task setup and the provision of expert knowledge. That does not mean that humans should be excluded from ML-based decision making, and there is certainly a necessary debate to be had about degrees of autonomy that are appropriate in various contexts. However, for the cases where society judges the benefits of automation outweigh the disadvantages, it is worth considering how AutonoML may be achieved.

Importantly, we do not profess the optimality of any particular AutonoML architecture. Given the breadth and malleability of the field, it is unlikely that any one framework proposal will perfectly subsume all

existing AutoML systems, let alone future advances. On the other hand, the merits and challenges of integration are best discussed with reference to concrete schematics. Thus, the literature survey in this monograph is accompanied by the graduated development of a conceptual framework, exemplifying the potential interplay between various elements of AutonoML. As a necessity, Section 2 lays the initial groundwork for this example architecture by considering the fundamentals of ML, abstracting and encapsulating them as the lowest level of automatic operations; this is where the ‘fit’ and ‘predict’ functionality displayed in Figure 1.1 resides.

The survey of AutoML begins in earnest within Section 3, which discusses the role of optimisation in automating the selection of an ML model/algorithm and associated hyperparameters. Section 4 then discards an assumption that the ML model need be monolithic, reviewing optimisation research for extended pipelines of data operators. This generalisation enables Section 5 to examine the optimisation of neural architectures specifically, while Section 6 focusses on the pre-processing elements of an ML pipeline, exploring the automation of feature engineering. Subsequently, Section 7 investigates how model search can be upgraded by meta-knowledge, leveraging information from external ML experiments, while Section 8 identifies the importance of ensembles and discusses how their management can be mechanised.

Notably, in terms of the ML workflow shown by Figure 1.2, the previously listed six sections focus heavily on the model-development phase – with a touch of data engineering – because this is the space in which the majority of AutoML research exists. Nonetheless, recent times have witnessed a significant broadening of scope along the entire workflow, and the next five sections document current research perspectives on the role of automation with respect to model deployment, model maintenance, and even problem formulation.

Thus, the paradigm of AutonoML is finally introduced in Section 9, defined by the ability to adapt models within dynamic contexts. This stimulates an examination within Section 10 of how the quality of any one solution should even be determined. Section 11 then examines the challenge of automating operations in low-resource settings, while Section 12 reviews efforts to reintegrate expert knowledge and user control

back into autonomous systems. The survey ends with an acknowledgment in Section 13 of the drive towards one-size-fits-all AutoML, i.e. the quest for general applicability. Finally, Section 14 concludes with a discussion on the overarching technical challenges of integration, while remaining cognisant of the fact that understanding and fostering general engagement with resulting technologies are complex endeavours in their own right.

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