Preface

The past decade has seen an explosion of machine learning research and applications; especially, deep learning methods have enabled key advances in many application domains, such as computer vision, speech processing, and game playing. However, the performance of many machine learning methods is very sensitive to a plethora of design decisions, which constitutes a considerable barrier for new users. This is particularly true in the booming field of deep learning, where human engineers need to select the right neural architectures, training procedures, regularization methods, and hyperparameters of all of these components in order to make their networks do what they are supposed to do with sufficient performance. This process has to be repeated for every application. Even experts are often left with tedious episodes of trial and error until they identify a good set of choices for a particular dataset.

The field of automated machine learning (AutoML) aims to make these decisions in a data-driven, objective, and automated way: the user simply provides data, and the AutoML system automatically determines the approach that performs best for this particular application. Thereby, AutoML makes state-of-the-art machine learning approaches accessible to domain scientists who are interested in applying machine learning but do not have the resources to learn about the technologies behind it in detail. This can be seen as a *democratization* of machine learning: with AutoML, customized state-of-the-art machine learning is at everyone's fingertips.

As we show in this book, AutoML approaches are already mature enough to rival and sometimes even outperform human machine learning experts. Put simply, AutoML can lead to improved performance while saving substantial amounts of time and money, as machine learning experts are both hard to find and expensive. As a result, commercial interest in AutoML has grown dramatically in recent years, and several major tech companies are now developing their own AutoML systems. We note, though, that the purpose of democratizing machine learning is served much better by open-source AutoML systems than by proprietary paid black-box services.

This book presents an overview of the fast-moving field of AutoML. Due to the community's current focus on deep learning, some researchers nowadays mistakenly equate AutoML with the topic of neural architecture search (NAS);

but of course, if you're reading this book, you know that – while NAS is an excellent example of AutoML – there is a lot more to AutoML than NAS. This book is intended to provide some background and starting points for researchers interested in developing their own AutoML approaches, highlight available systems for practitioners who want to apply AutoML to their problems, and provide an overview of the state of the art to researchers already working in AutoML. The book is divided into three parts on these different aspects of AutoML.

Part I presents an overview of AutoML methods. This part gives both a solid overview for novices and serves as a reference to experienced AutoML researchers.

Chap. 1 discusses the problem of hyperparameter optimization, the simplest and most common problem that AutoML considers, and describes the wide variety of different approaches that are applied, with a particular focus on the methods that are currently most efficient.

Chap. 2 shows how to *learn to learn*, i.e., how to use experience from evaluating machine learning models to inform how to approach new learning tasks with new data. Such techniques mimic the processes going on as a human transitions from a machine learning novice to an expert and can tremendously decrease the time required to get good performance on completely new machine learning tasks.

Chap. 3 provides a comprehensive overview of methods for NAS. This is one of the most challenging tasks in AutoML, since the design space is extremely large and a single evaluation of a neural network can take a very long time. Nevertheless, the area is very active, and new exciting approaches for solving NAS appear regularly.

Part II focuses on actual AutoML systems that even novice users can use. If you are most interested in applying AutoML to your machine learning problems, this is the part you should start with. All of the chapters in this part evaluate the systems they present to provide an idea of their performance in practice.

Chap. 4 describes Auto-WEKA, one of the first AutoML systems. It is based on the well-known WEKA machine learning toolkit and searches over different classification and regression methods, their hyperparameter settings, and data preprocessing methods. All of this is available through WEKA's graphical user interface at the click of a button, without the need for a single line of code.

Chap. 5 gives an overview of Hyperopt-Sklearn, an AutoML framework based on the popular scikit-learn framework. It also includes several hands-on examples for how to use system.

Chap. 6 describes Auto-sklearn, which is also based on scikit-learn. It applies similar optimization techniques as Auto-WEKA and adds several improvements over other systems at the time, such as meta-learning for warmstarting the optimization and automatic ensembling. The chapter compares the performance of Auto-sklearn to that of the two systems in the previous chapters, Auto-WEKA and Hyperopt-Sklearn. In two different versions, Auto-sklearn is the system that won the challenges described in Part III of this book.

Chap. 7 gives an overview of Auto-Net, a system for automated deep learning that selects both the architecture and the hyperparameters of deep neural networks. An early version of Auto-Net produced the first automatically tuned neural network that won against human experts in a competition setting.

Chap. 8 describes the TPOT system, which automatically constructs and optimizes tree-based machine learning pipelines. These pipelines are more flexible than approaches that consider only a set of fixed machine learning components that are connected in predefined ways.

Chap. 9 presents the Automatic Statistician, a system to automate data science by generating fully automated reports that include an analysis of the data, as well as predictive models and a comparison of their performance. A unique feature of the Automatic Statistician is that it provides natural-language descriptions of the results, suitable for non-experts in machine learning.

Finally, Part III and Chap. 10 give an overview of the AutoML challenges, which have been running since 2015. The purpose of these challenges is to spur the development of approaches that perform well on practical problems and determine the best overall approach from the submissions. The chapter details the ideas and concepts behind the challenges and their design, as well as results from past challenges.

To the best of our knowledge, this is the first comprehensive compilation of all aspects of AutoML: the methods behind it, available systems that implement AutoML in practice, and the challenges for evaluating them. This book provides practitioners with background and ways to get started developing their own AutoML systems and details existing state-of-the-art systems that can be applied immediately to a wide range of machine learning tasks. The field is moving quickly, and with this book, we hope to help organize and digest the many recent advances. We hope you enjoy this book and join the growing community of AutoML enthusiasts.

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