AutoML: Introduction

Risks of AutoML

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Risks of AutoML

1. Users apply AutoML without understanding anything.
   - Users might wonder why (Auto-)ML does not perform well after they passed in poor data.

Risks of AutoML

2. Users trust AutoML too much.
   - humans might not use human reasoning skills and do not second guess machine decisions

Risks of AutoML

3. We enable non-ML experts to use ML
   without knowing the risks and consequences of ML.
   - E.g., bias in data and trained models

Risks of AutoML

4. Could result in deployment of ...

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   - inaccurate models due to lack of understanding of statistical concepts, e.g., sampling bias, overfitting, concept drift, ...
   - biased and unfair models due to lack of understanding ethical practices and use of features such as gender and race for predicting outcomes

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2. Build systems that automatically warn of these risks
   - AutoML should go hand in hand in bias analysis
   - ⇝ Future research topics (as of March 2020)
3. Can we automatically find ML systems that are less prone to such risks?
   - ⇝ Future research topics (as of March 2020)

AutoML: Introduction

How is Everything connected?

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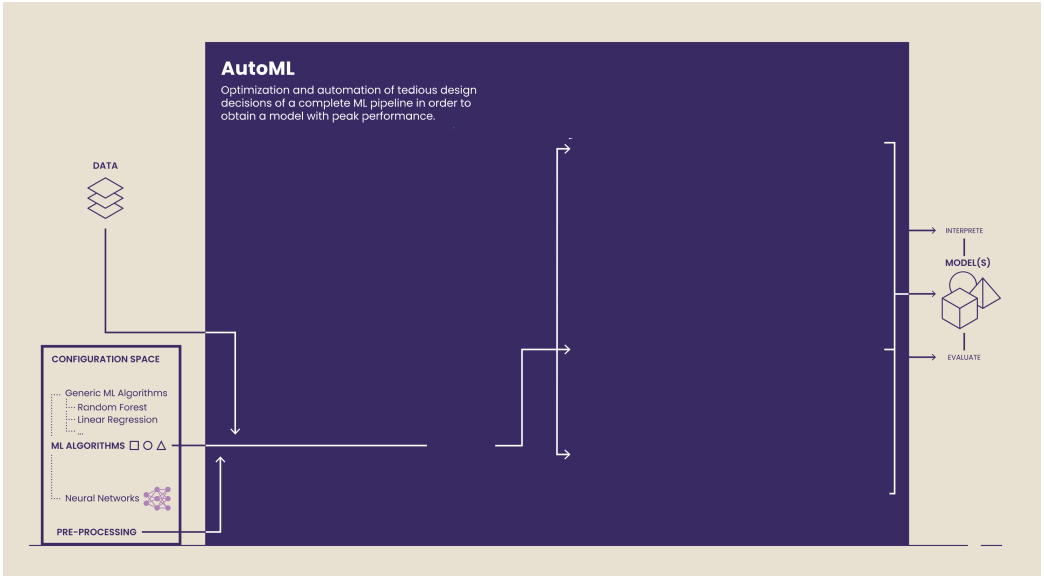
Building a Successful AutoML Tool

$\rightsquigarrow$ There is not a single way for building successful AutoML tools, but there are well established ideas.

- Hyperparameter optimization
- Neural architecture search
- Model and algorithm selection
- Dynamic approaches

$\rightsquigarrow$ But how can we combine all of these?

AutoML


AutoML
Optimization and automation of tedious design decisions of a complete ML pipeline in order to obtain a model with peak performance.
DATA
CONFIGURATION SPACE
Generic ML Algorithms
Random Forest
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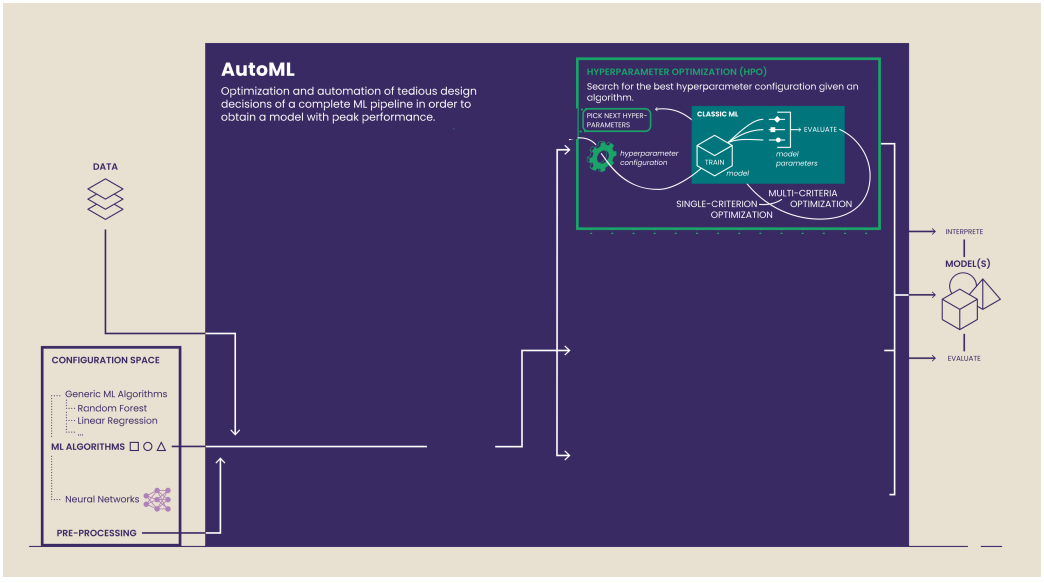
...
ML ALGORITHMS
Neural Networks
PRE-PROCESSING
INTERPRETE
MODEL(S)
EVALUATE

AutoML + HPO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HYPERPARAMETER OPTIMIZATION (HPO)
Search for the best hyperparameter configuration given an algorithm.
PICK NEXT HYPER-PARAMETERS
hyperparameter configuration
CLASSIC ML
TRAIN
model
EVALUATE
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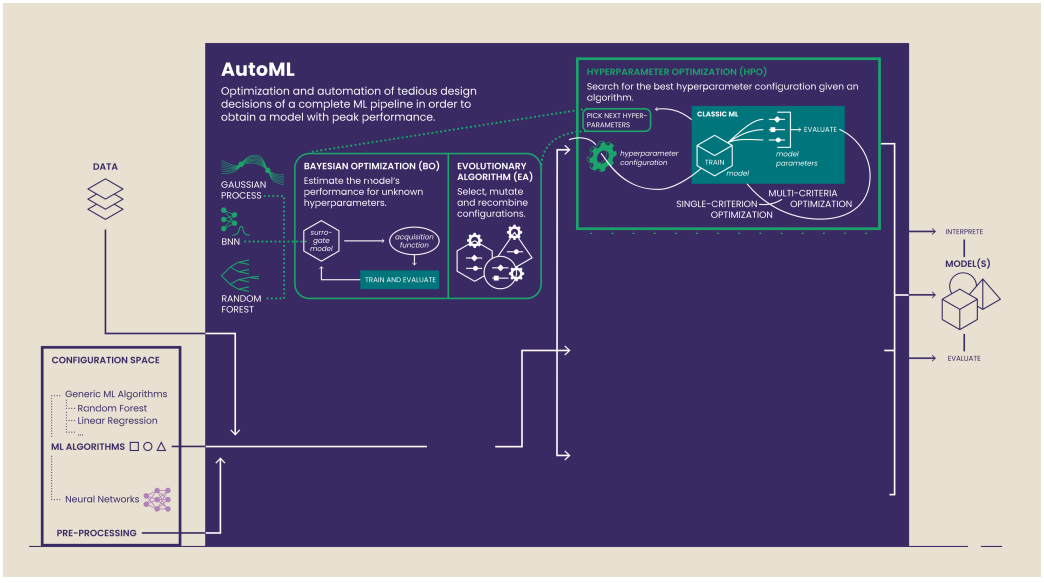
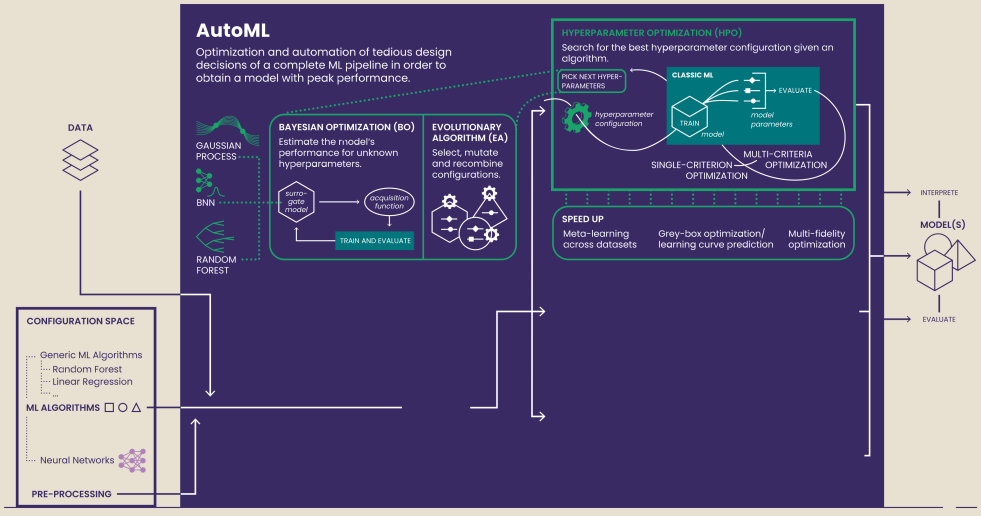
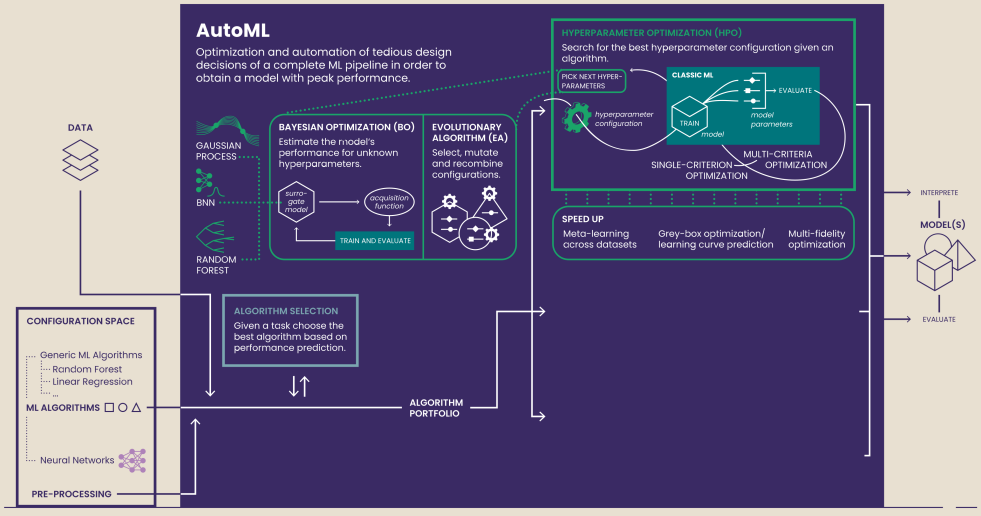
AutoML + HPO + BO



AutoML + HPO + BO + Speed up



AutoML + HPO + BO + Speed up + AS



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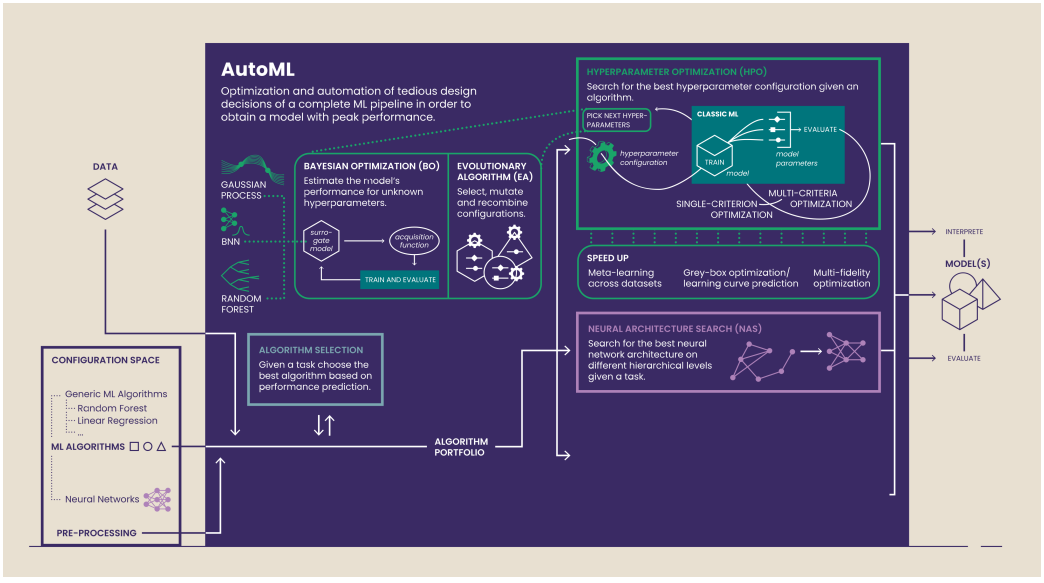

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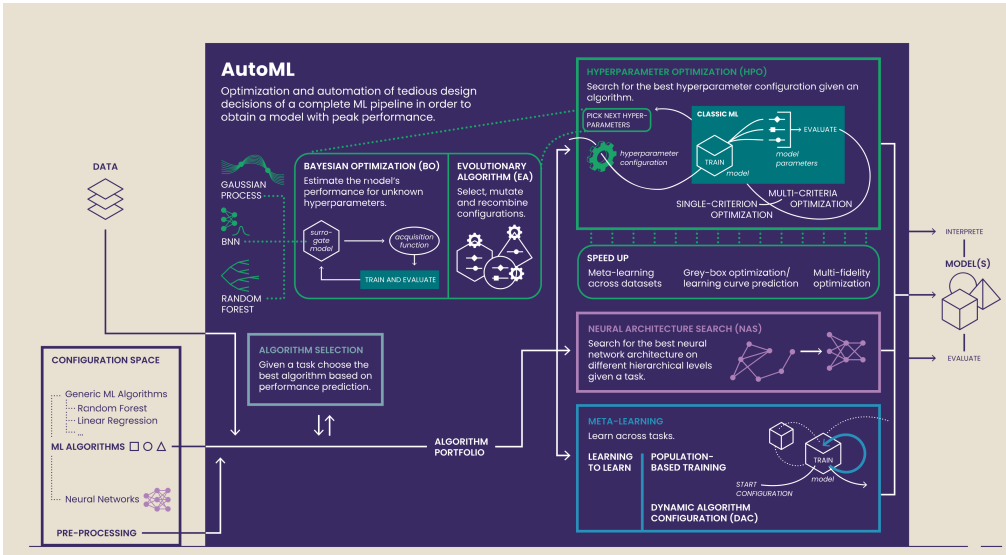

AutoML: Introduction

The Big Picture

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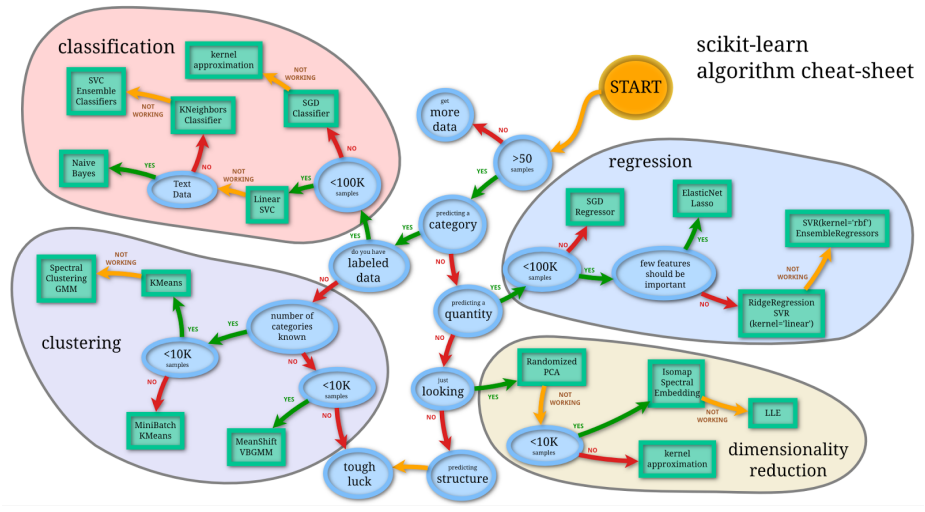
Machine Learning

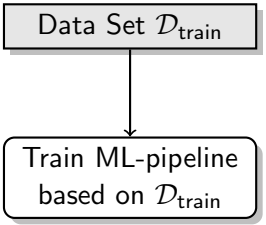
"Machine learning is the science of getting computers to act without being explicitly programmed."

by Andrew Ng

Machine Learning requires many design decisions



Machine Learning Workflow



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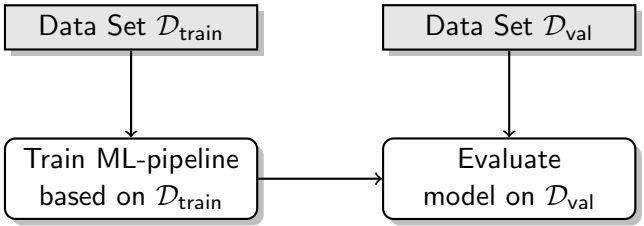

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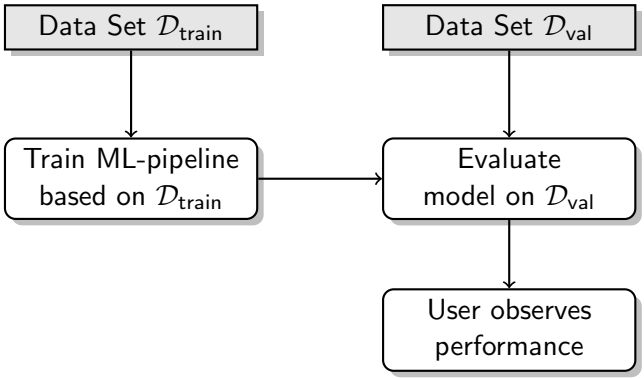

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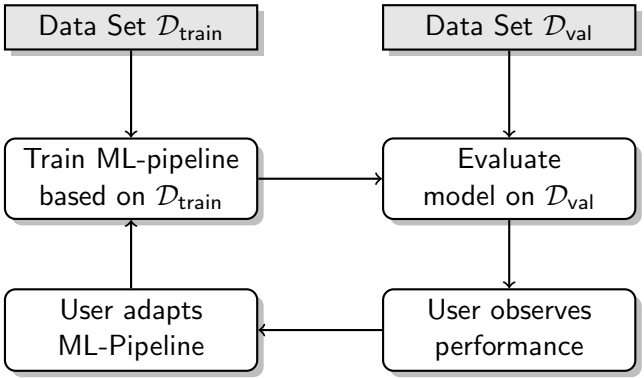

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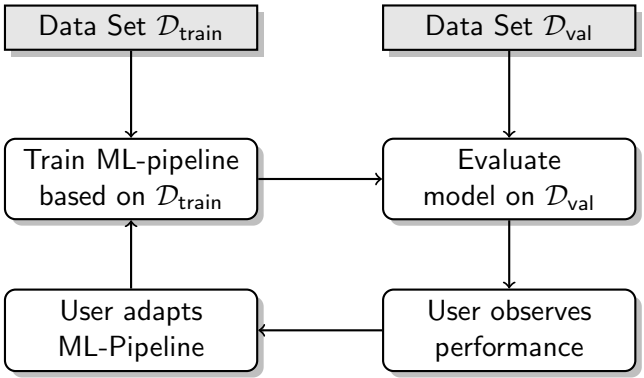

$\rightsquigarrow$ Users indirectly teach machines how to learn.

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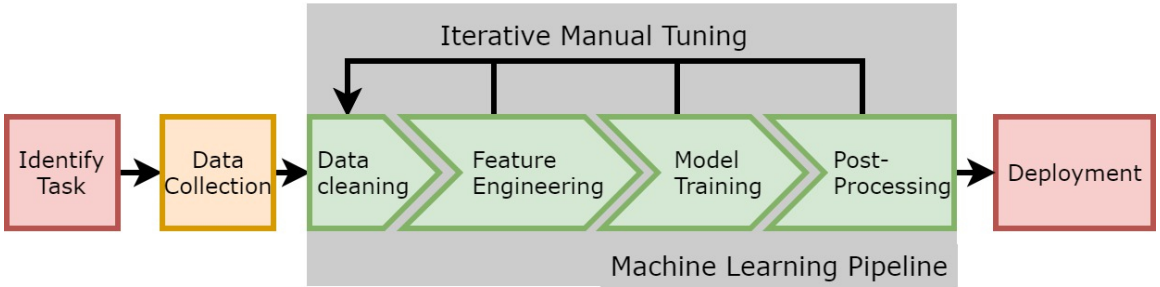
Zoubin Ghahramani said that he often heard that:

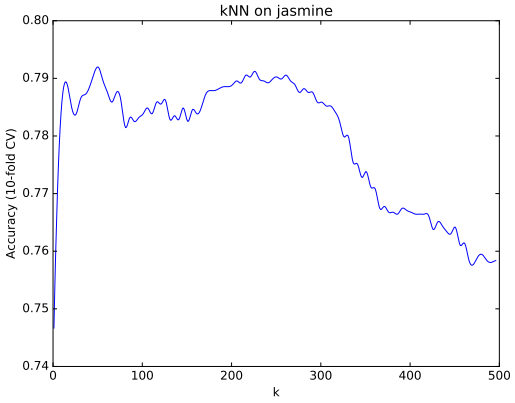
"I'd like to use machine learning, but I can't invest much time."

Why does ML development take a lot of time?



$\rightsquigarrow$ To achieve state-of-the-art performance,
this manual tuning has to be done for each new dataset again.

A Simple Example with k-NN



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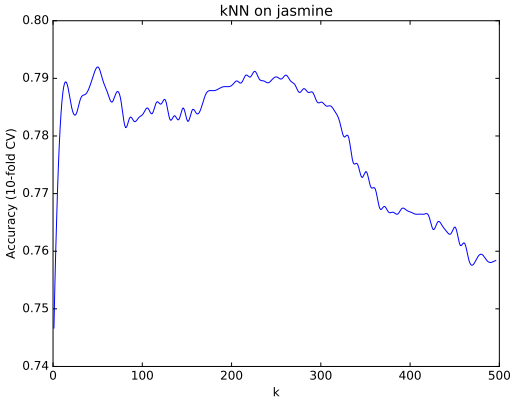

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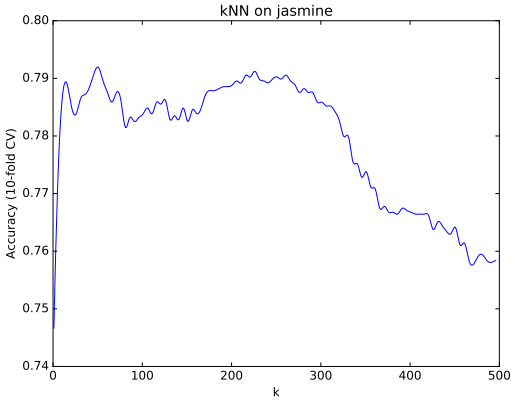

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- Size of neighbourhood (k) is very important for its performance
- The performance function depending on k is quite complex (not at all convex)

Goal of AutoML

AutoML

The goal of AutoML is to automate all parts of machine learning
(as needed) to *support* users efficiently building their ML-applications.

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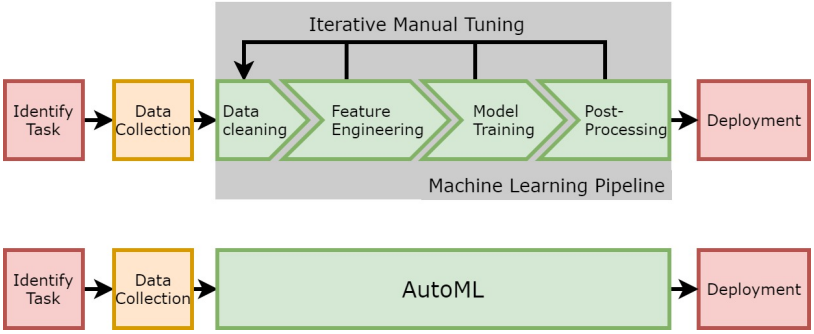
Informal Definition: AutoML System

Given

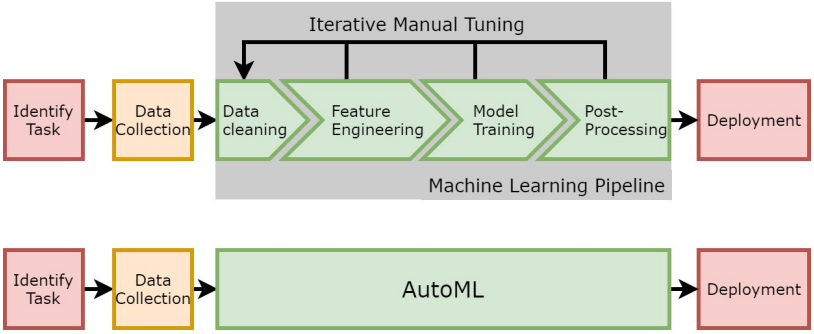
- a dataset
- a task (e.g., regression or classification)
- a cost metric (e.g., accuracy or RMSE)

an AutoML system automatically determines the approach that performs best for this particular application.

ML vs AutoML


Iterative Manual Tuning
Identify Task
Data Collection
Data cleaning
Feature Engineering
Model Training
Post-Processing
Deployment
Machine Learning Pipeline
Identify Task
Data Collection
AutoML
Deployment

ML vs AutoML



With AutoML, we ...

- support ML users
- improve the efficiency of developping new ML applications
- reduce the required ML-expertise
- might achieve better performance than developers w/o AutoML

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4. broader use of ML also in other disciplines
   - ML should not be limited to computer scientists;
   - the most amazing applications of ML are often done by either interdisciplinary teams or even non-computer scientists

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4. optimization in highly complex spaces
   - incl. categorical choices, continuous parameters, conditional dependencies

AutoML: Introduction

Overview of AutoML Problems

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Objectives of AutoML

Different metrics to measure the success of ML and AutoML:

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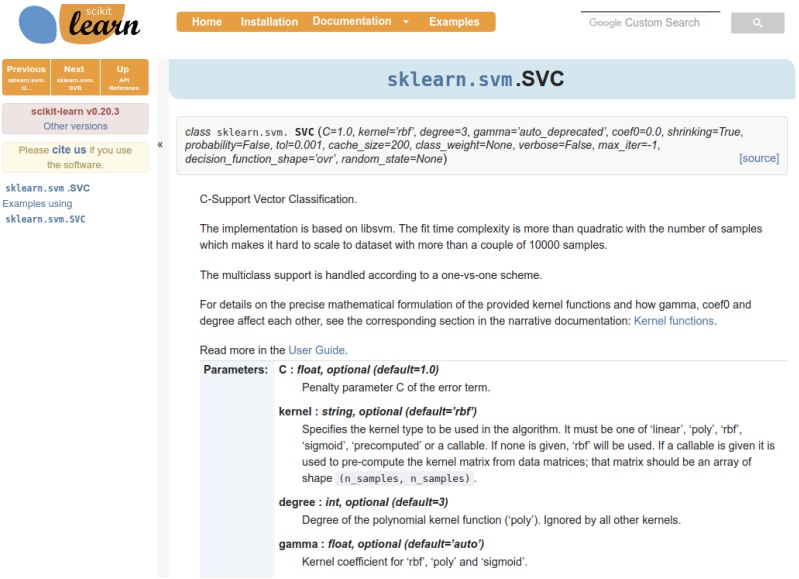
$\rightsquigarrow$ AutoML optimizes an arbitrary cost function, denoted as c.

$\rightsquigarrow$ $c(\cdot)$ can also return several cost metrics

Hyperparameters of an SVM



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- Sometimes, we want to optimize for different metrics, instead of one
  - $\rightsquigarrow$ multi-objective optimization and Pareto fronts

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  - ...
- studied 179 classifiers on 121 datasets [Fernández-Delgado et al. 2015]
- In practice, we actually want to jointly choose the best ML-algorithm and its hyperparameters

CASH: Combined Algorithm Selection and Hyperparameter Optimization

Definition

Let

- $\mathbf{A} = \{\mathcal{A}_1, \mathcal{A}_2, \ldots, \mathcal{A}_k\}$ be a set of algorithms (a.k.a. portfolio)
- $\mathbf{\Lambda}$ be a set of hyperparameters of each machine learning algorithm $\mathcal{A}_i$
- $\mathcal{D}_{opt}$ be a dataset which is split into $\mathcal{D}_{train}$ and $\mathcal{D}_{valid}$
- $c(\mathcal{A}_{\boldsymbol{\lambda}}, \mathcal{D}_{train}, \mathcal{D}_{valid})$ denote the cost of $\mathcal{A}_{\boldsymbol{\lambda}}$ trained on $\mathcal{D}_{train}$ and evaluated on $\mathcal{D}_{valid}$.

we want to find the best combination of algorithm $\mathcal{A} \in \mathbf{A}$ and its hyperparameter configuration $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ minimizing:

$$(\mathcal{A}^*, \boldsymbol{\lambda}^*) \in \underset{\mathcal{A} \in \mathbf{A}, \boldsymbol{\lambda} \in \mathbf{\Lambda}}{\arg\min}\, c(\mathcal{A}_{\boldsymbol{\lambda}}, \mathcal{D}_{train}, \mathcal{D}_{valid})$$

Architectures of Neural Networks

- Many architecture were proposed
- Differences in
  - Depth
  - Resolution
  - Width
  - Operators
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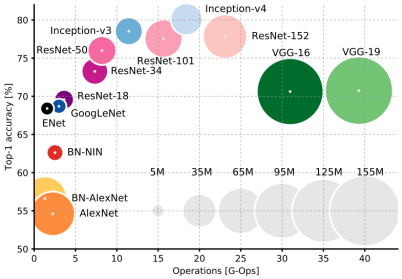
  - ...



on Imagenet [Canzian et al. 2017]

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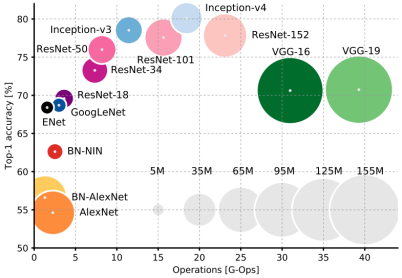

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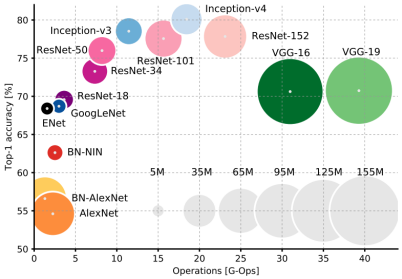

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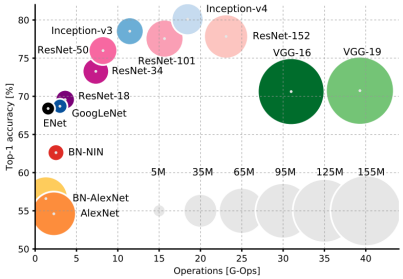

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- Already on a single dataset such as ImageNet, it is not obvious which architeture to choose
- For other datasets, you might need different architectures to achieve top-performance
  - For similar datasets, you might use scaled versions of known architectures (e.g., CIFAR10 and Imagenet)

Neural Architecture Search (NAS)

Definition

Let

- $\boldsymbol{\lambda}$ be an architecture for a deep neural network N with domain $\boldsymbol{\Lambda}$,
- $\mathcal{D}_{opt}$ be a dataset which is split into $\mathcal{D}_{train}$ and $\mathcal{D}_{valid}$
- $c(N_{\boldsymbol{\lambda}}, \mathcal{D}_{train}, \mathcal{D}_{valid})$ denote the cost of $N_{\boldsymbol{\lambda}}$ trained on $\mathcal{D}_{train}$ and evaluated on $\mathcal{D}_{valid}$.

The *neural architecture search (NAS)* problem is to find an architecture that minimizes this cost:

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Remark:

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- In practice, you want jointly optimize HPO and NAS [Zela et al. 2018]

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- For solving the HPO, CASH and NAS problem, we use some kind of optimization approach to search for a solution

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the *per-instance algorithm selection problem* is to obtain a mapping $s : \mathcal{D} \mapsto \mathcal{A}$ such that

$$\arg\min_{s} \int_{\mathbf{D}} c(s(\mathcal{D}), \mathcal{D}) p(\mathcal{D}) \, \mathrm{d}\mathcal{D}$$

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the *dynamic algorithm configuration problem (DAC)* is to obtain a configuration policy $\pi^* : s_t \times \mathcal{D} \mapsto \boldsymbol{\lambda}$ by optimizing its cost across a distribution of datasets:

$$\pi^* \in \arg\min_{\pi \in \mathbf{\Pi}} \int_{\mathbf{D}} p(\mathcal{D}) c(\pi, \mathcal{D}) \, \mathrm{d}\mathcal{D}$$

Summary

HPO	Search for the best hyperparameter configuration of a ML algorithm
CASH	Search for the best combination of algorithm and hyperparameter configuration
NAS	Search for the architecture of neural network
Selection	Predict the best algorithm (and its hyperparameter configuration)
DAC	Predict the best hyperparameter configuration for an algorithm state at a given time point

AutoML: Introduction

The Team

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- Head of the statistical learning and data science group
- Co-Director of Munich Center for Machine Learning
- Founder of MLR (Machine Learning in R)
- Co-Founder of `www.openml.org`
- Co-Founder and advisory board member of COSEAL
  (Configuration and Selection of Algorithms)

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- Professor at
  the University of Freiburg (Germany)
- Head of the machine learning lab
- Won 1st and 2nd international AutoML challenge
- Co-author of popular AutoML tools Auto-WEKA,
  Auto-sklearn, Auto-PyTorch
- Co-founder and co-organizer of AutoML workshop series at
  ICML (since 2014)
- Co-Editor of book on *Automated Machine Learning:
  Methods, Systems, Challenges*
- Co-Head of `automl.org`

Lars Kotthoff

- Professor at
  the University of Wyoming (USA)
- Head of the Meta-Algorithmics, Learning and Large-Scale Empirical Testing lab (MALLET) and director of the Artificially Intelligent Manufacturing Center (AIM)
- Developer of MLR (Machine Learning in R)
- Organizer of competitions on algorithm selection
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Marius Lindauer

- Professor at
  the Leibniz University of Hannover (Germany)
- Head of the machine learning group
- Won 1st and 2nd international AutoML challenge
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Janek Thomas

- Group Lead for AutoML & XAI at Fraunhofer IIS
- Phd from the Ludwig-Maximilians-University Munich (Germany)
- Developer of MLR, the amlb AutoML benchmark and autoxgboost
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- Professor at
  Eindhoven University of Technology (Netherlands)
- Machine learning, Meta-Learning
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- Julia Moosbauer
- Jakob Richter
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- Arber Zela

... and many more