Automated Machine Learning (AutoML)

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Motivation

- 1. Machine learning is very successful
- 2. To build a traditional ML pipeline:
 - Domain experts with longstanding experience
 - Specialized data preprocessing
 - > Domain-driven meaningful feature engineering
 - Picking right models
 - Hyper-parameter tuning
 - **>**

AutoML Vision

For Non-Experts

AutoML allows non-experts to make use of machine learning models and techniques without requiring to become an expert in this field first

https://en.wikipedia.org/wiki/Automated_machine_learning

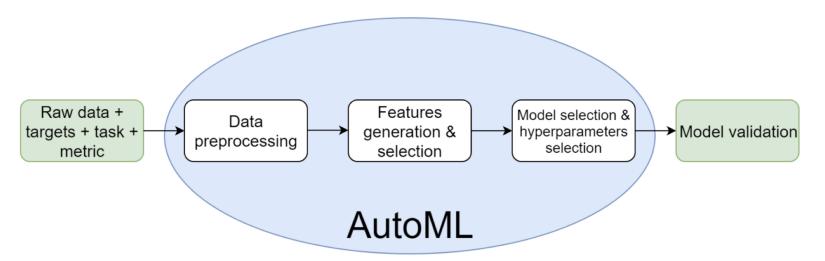
For Data Scientists

AutoML aims to augment, rather than automate, the work and work practices of heterogeneous teams that work in data science.

Wang, Dakuo, et al. "Human-Al Collaboration in Data Science: Exploring Data Scientists' Perceptions of Automated Al." Proceedings of the ACM on Human-Computer Interaction 3.CSCW (2019): 1-24.

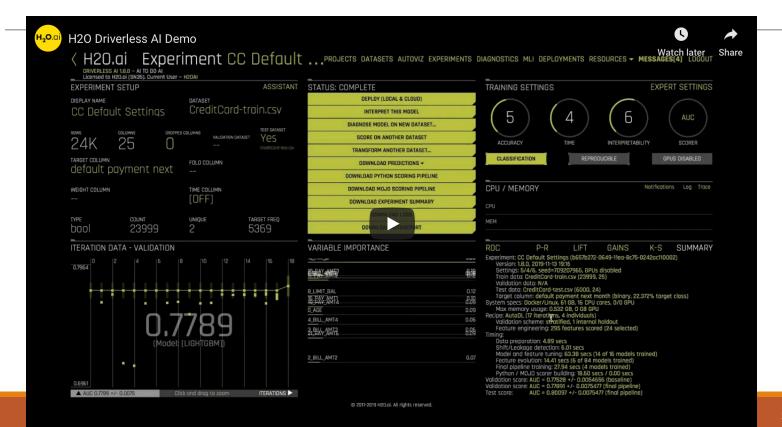
What is AutoML?

Automate the process of applying machine learning to realworld problems



H20 Driverless Al Demo

https://www.youtube.com/watch?v=ZqCoFp3-rGc



Outline

Auto Feature Selection (Lecture 6)

Auto Hyperparameter Tuning (Lecture 6)

Auto Feature Generation (This Lecture)

Neural Architecture Search (This Lecture)

Auto Feature Generation

Motivation

- The model performance is heavily dependent on quality of features in dataset
- It's time-consuming for domain experts to generate enough useful features



Feature Generation

- Unary operators (applied on a single feature)
 - Discretize or normalize numerical features
 - Apply rule-based expansions of dates
 - Mathematical operators (e.g., Log Function)
- Higher-order operators (applied on 2+ features)
 - Basic arithmetic operations (e.g., +, -, ×, ÷)
 - Group-by Aggregation (e.g., GroupByThenMax, GroupByThenMin)

Featuretools



An open source library for performing automated feature engineering

Design to fast-forward feature generation across multi-relational tables

Concepts

- Entity is the relational tables
- An EntitySet is a collection of entities and the relationships between them
- Feature Primitives
 - Unary Operator: transformation (e.g., MONTH)
 - High-order Operator: Group-by Aggregation (e.g., GroupByThenSUM)

Entity sets

Customer

Product

Customer_id	Birthdate	MONTH(Birthdate)	SUM(Product.Price)
1	1995-09-28	9	\$500
2	1980-01-01	1	
3	1999-02-02	2	

GroupBy ThenSUM:

Product_id	Customer_id	Name	Price
1	1	Banana	\$100
2	1	Banana	\$100
3	1	Orange	\$300
4	2	Apple	\$50
			•••

Unary Operator:

MONTH -

Feature Primitives

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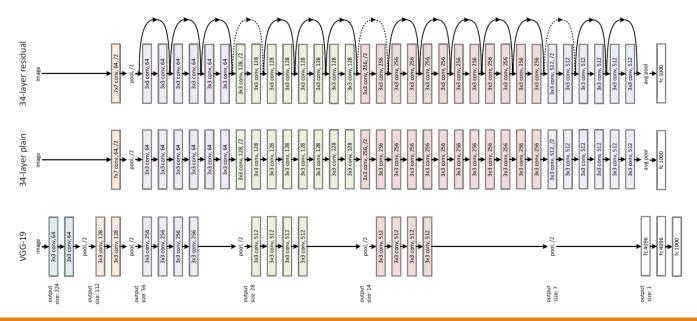
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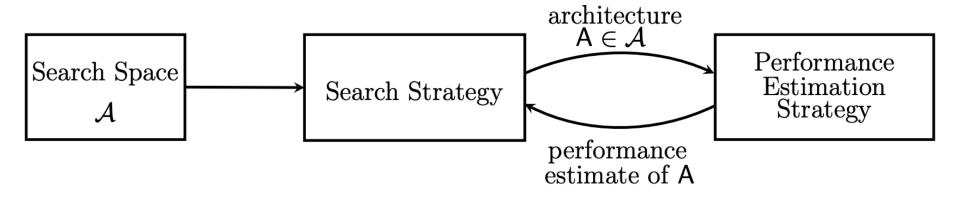
Neural Architecture Search (NAS)

Motivation

How can someone come out with such an architecture?

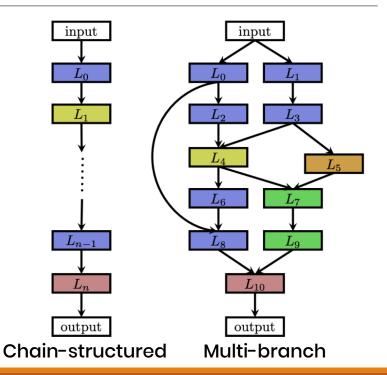


Neural Architecture Search: Big Picture



Search Space

- Define which neural architectures a NAS approach might discover in principle
- ♦ May have human bias → prevent finding novel architectural building blocks



Search Strategy

Basic Idea

> Explore search space (often exponentially large or even unbounded)

Methods

- Random Search
- Evolutionary Methods [Angeline et al., 1994]
 Bayesian Optimization [Bergstra et al., 2013]
- Reinforcement Learning [Baker et al., 2017]

Performance Estimation Strategy

Basic Idea

The process of estimating predictive performance

Methods

- Simplest option: perform a training and validation of the architecture on data
- Initialize weights of novel architecture based on weights of other architectures have been trained before
- Using learning curve extrapolation [Swersky et al., 2014]
- **>**

Summary

What is AutoML and why we need it? How AutoML works?

- Auto Feature Selection (Lecture 6)
- Auto Hyperparameter Tuning (Lecture 6)
- Auto Feature Generation (This Lecture)
- Neural Architecture Search (This Lecture)