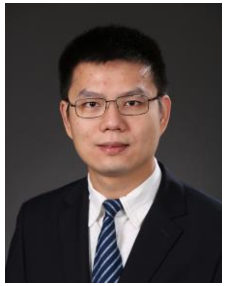
Automated Recommender System (RecSys)

Quanming Yao[1,2], Yong Li[1], Chen Gao[1], Huan Zhao[2], Yongqi Zhang[2]

[1]*Department of Electronic Engineering, Tsinghua University*

[2]*4Paradigm Inc.*

https://quanmingyao.github.io/AutoML.github.io/ijcai21-tutorial.html





Tutorial Outline

1. An introduction to Automated Machine Learning (AutoML)
   - Background on technical tools from machine learning
2. Why AutoML is Needed in RecSys and Recent Advances
   - Exemplar works introducing AutoML into RecSys
3. Automated Graph Representation Learning for RecSys
   - Explore neural architecture search for GNN based RecSys
4. Automated Knowledge Graph (KG) Embedding
   - Explore AutoML for KG Embedding based RecSys

Schedule at a Glance

Time	Event
0:00-0:40 minutes	**Part 1**: An introduction to Automated Machine Learning (AutoML)
	Speaker: Quanming Yao
0:40-1:20 minutes	**Part 2**: Why AutoML is Needed in RecSys and Recent Advances
	Speaker: Chen Gao
1:20-1:30 minutes	**Break**
1:30-2:10 minutes	**Part 3**: Automated Graph Neural Network for RecSys
	Speaker: Huan Zhao
2:10-2:50 minutes	**Part 4**: Automated Knowledge Graph Embedding
	Speaker: Yongqi Zhang
2:50-3:00 minutes	**Part 5**: Discussion

Automated Recommender System (RecSys) Tutorial

Part 1: An Introduction to Automated Machine Learning (AutoML)

Quanming Yao[1,2]

[1]*Assistant professor - Department of Electronic Engineering, Tsinghua University*

[2]*Founding Leader (ML research team), 4Paradigm Inc.*

qyaoaa@tsinghua.edu.cn

Outline

1. What is Machine Learning?
2. What is Automated Machine Learning (AutoML)?
3. Summary & Next Works

What is Machine Learning (ML)?

Applications

Search Engine
Recommender Systems
Loss Assessment

Image Classification

Predict the class of the object

Security Monitoring
Bio-payment
Flow Statistics

Face Recognition

Who is the person

COVID Simulation
Petroleum Exploration
Drug Discovery

Drug Design

Learn to make decisions

Better Performance

Higher Efficiency

Definition

Structure Samples

$$\boxed{\min_x F(\,x\,;D\,)} \xrightarrow[\text{optimization}]{\text{(iterative)}} \text{Prediction Accuracy} \uparrow$$

Parameters

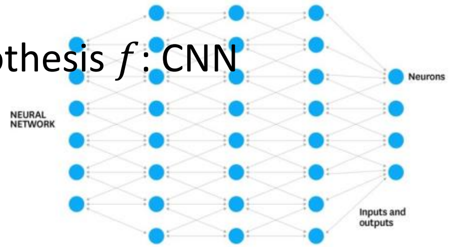
[1]. Machine Learning, Tom Mitchell, McGraw Hill, 1997.
[2]. 周志华 著. 机器学习, 北京: 清华大学出版社, 2016年

ML = Data + Knowledge

Image Classification

Optimization ⇩

Hypothesis f: CNN



Generalization ⇩

Accuracy

Design a **hypothesis (function) f** to perform the learning task

Target	Concept	Issue
Better Performance (more important) →	Generalization →	What kind of f should we use?
Higher Efficiency →	Optimization →	How can we find such f?

Not everything can be learnt

PAC-Learning (Definition 2.3 in [1]): What kind of problems can be solved in polynomial time

No Free Lunch Theorem (Appendix B [2]): No single algorithm can be good on all problems

[1]. M. Mohri, A. Rostamizadeh, A. Talwalkar. Foundations of machine learning. 2018
[2]. O. Bousquet, et.al. Introduction to Statistical Learning Theory. 2016

How to use ML Well?

Prior Knowledge

Optimization

Data

Hypothesis Model

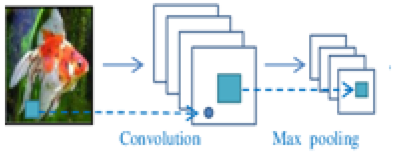
Generalization Performance

The Advancement of Learning

- An iteration between theory and practice

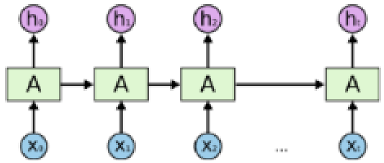
- A feedback loop

CNN

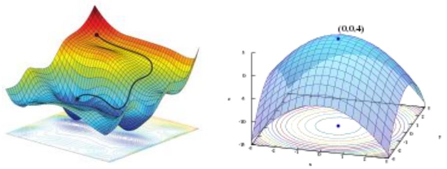


/

RNN



Generalization: What kind of f should we use?



SGD v.s. Adagrad[1]

Optimization: How can we find such f?

Prior knowledge

“All models are wrong, but some are useful”[2]

Better understanding of prior knowledge → Better hypothesis → Better generalization performance

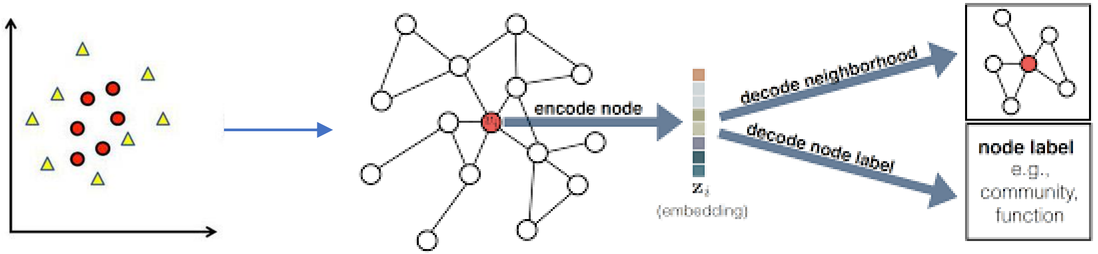
[1]. Image Source: A. Amini et al. “Spatial Uncertainty Sampling for End-to-End Control”. NeurIPS Bayesian Deep Learning 2018
[2]. G. Box, Science and statistics, JASA 1976

Continual Trends in Machine Learning

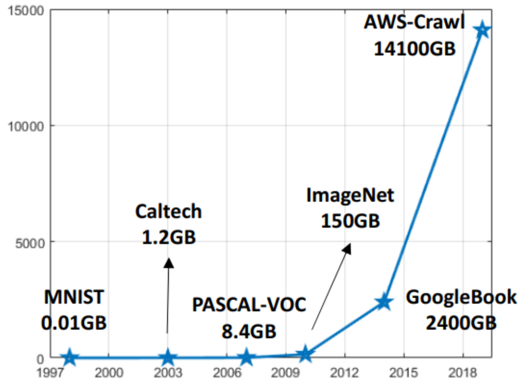
Given Task

$\min_x F(x; D)$

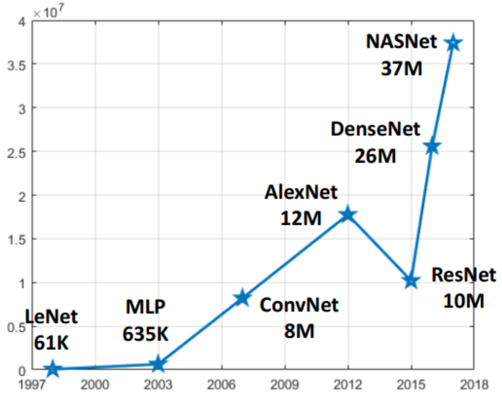
F: More Complicated Structure



D: More Samples



x: More Parameters



Moving Direction

Stronger models → better performance

Road Map in Recent History

- Core Issue in Machine Learning: Improving learning performance (with higher efficiency)

Rule-based
association rules mining, learning classifier systems
1990s

Statistics-based
support vector machine, sparse dictionary learning
2000s

Deep Learning-based
convolutional neural networks, transformer
2010s

Better performance

- Larger hypothesis (more complex models) are being used
- Optimization is getting complex (even mixed up with generalization)
- The prior knowledge is imposed on more abstract level

What is ML – Summary

- Machine learning = Data (optimization) + Knowledge (generalization)
  - Core Issue: Improving learning performance (with high efficiency)
- The advance and usage of ML is an iterative process
  - Better understanding of prior knowledge → Better generalization performance
- Continual trends in machine learning
  - The prior knowledge is imposed on more abstract level

Outline

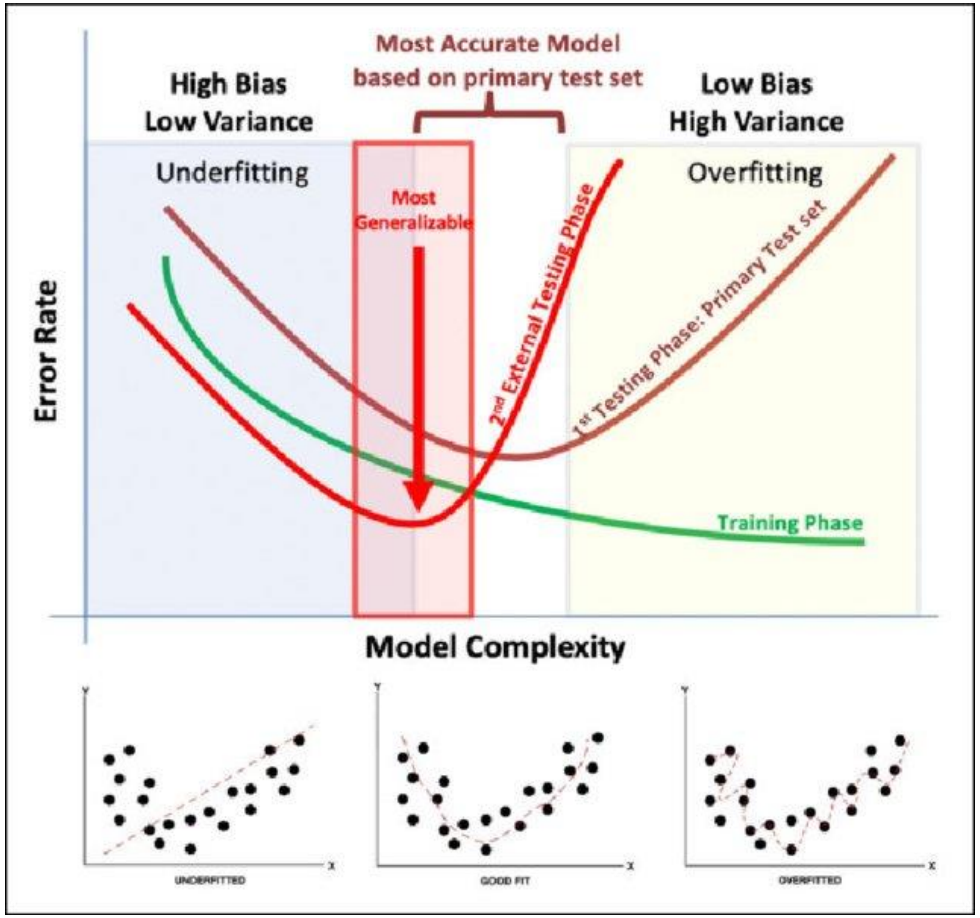
1. What is Machine Learning?
2. What is Automated Machine Learning (AutoML)?
   - Explanation from a Simple Example
   - Recent Industrial and Research Examples
   - A Generalization Viewpoint for AutoML
   - How to use AutoML
3. Summary & Next Works

Simple Example – Tune hyper-parameter

$\boxed{\text{Bi-level optimization}}$

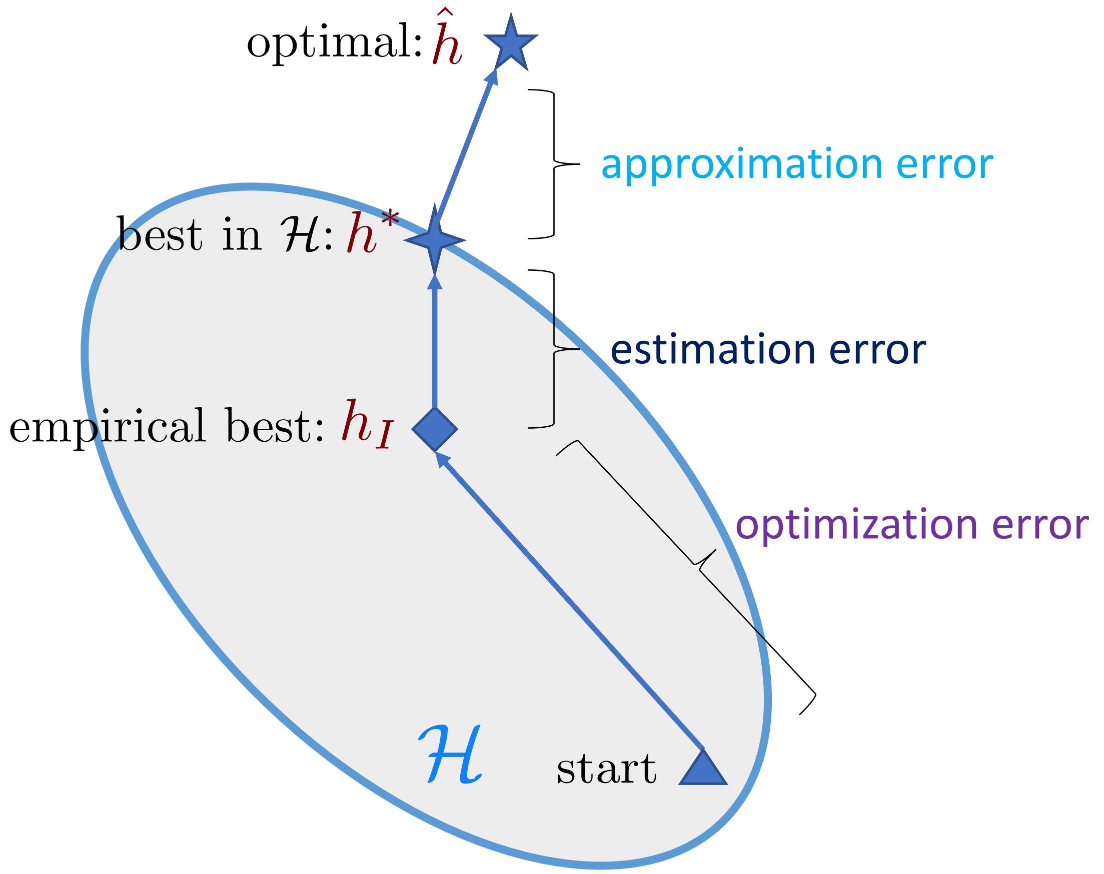
$$\underbrace{\max_{\lambda} \sum_{j} h(x_j; w^*)}_{\text{Validation Performance}} \quad \text{s.t.} \quad w^* = \underbrace{\min_{w} \sum_{i} f(x_i; w) + \overset{\text{Hyper-parameter}}{\lambda} \|w\|_1}_{\text{Training objective}}$$

- Large λ leads to sparse w^*
- Grid search: enumerating $\lambda \in \{1,2,4,8, \dots\}$



[1]. Image source: Artificial Intelligence and Machine Learning in Pathology: The Present Landscape of Supervised Methods.

Mach. Learn – Error decomposition



Total error in machine learning

- Approximation error
  - Which classifier to be used
  - What are their hyper-parameters
  - Distribution changes
- Estimation error
  - Finite samples
  - Regularization hyper-parameter

Reduce

$$\min_{w} \sum_{i} f(x_i; w) + \lambda \|w\|_1$$

- Optimization error
  - Which algorithm to be used
  - How to tune its step-size

Image is from Y. Wang, et. al. Generalizing from a Few Examples: A Survey on Few-Shot Learning. CSUR 2020

Look Inside Error Decomposition

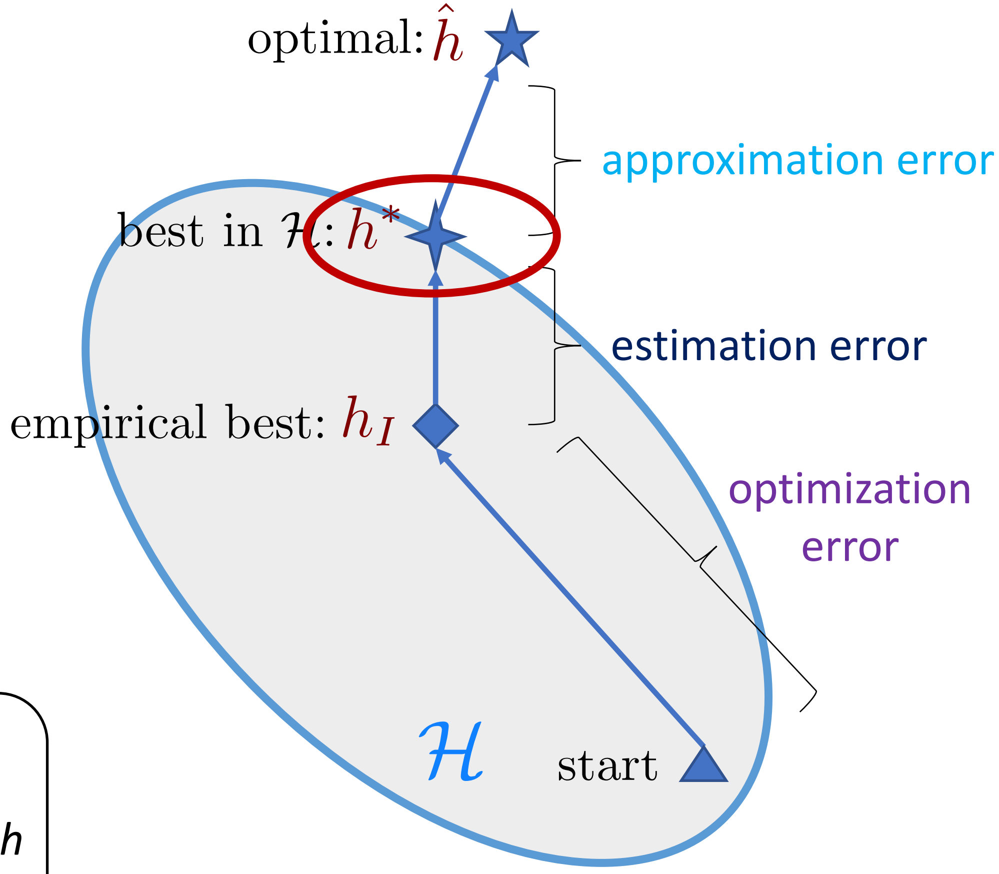
Automatically find h^* by bi-level optimization

$$\underbrace{\max_{\lambda} \sum\nolimits_j h(x_j; w^*)}_{\text{Validation Performance}} \quad \text{s.t.} \quad w^* = \underbrace{\min_{w} \sum\nolimits_i f(x_i; w) + \lambda \|w\|_1}_{\text{Training objective}}$$

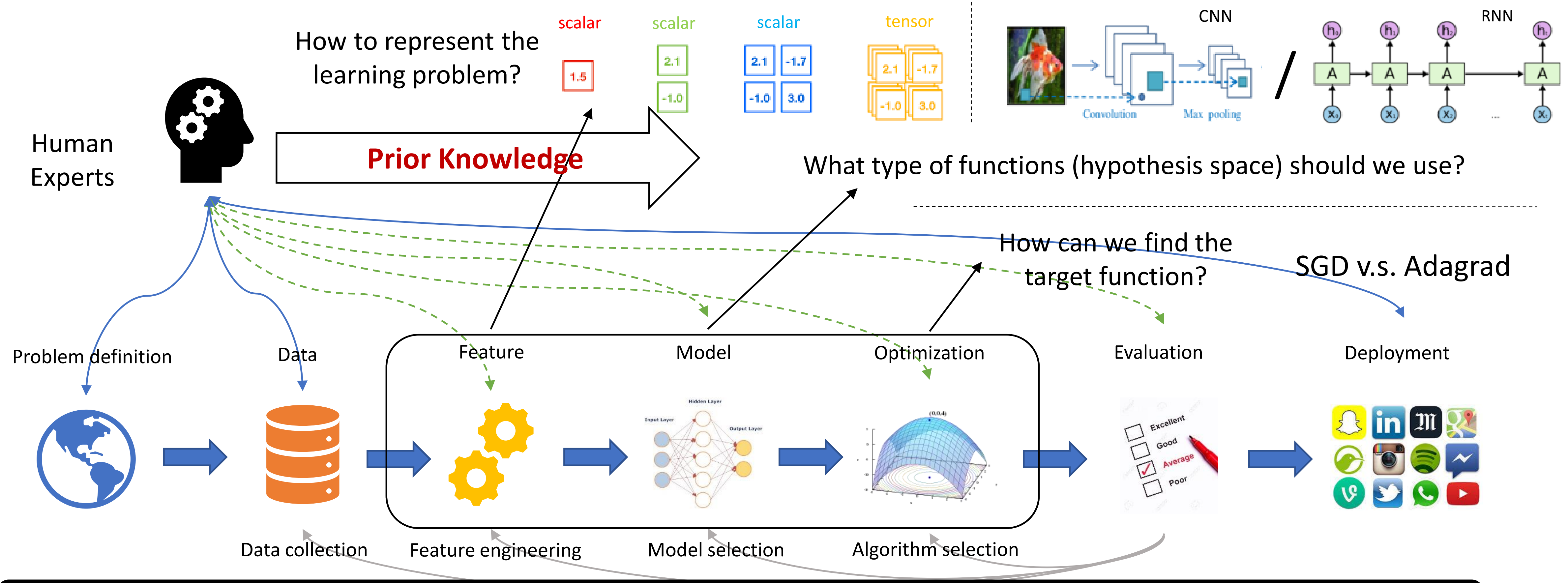
How to further improve the performance in an automatic manner (i.e., reduce the approximation error)?

- Feature can be weak → *Automatic feature engineering*
- Linear predictor can be too restrictive → *Neural architecture search*
- Grid search can be slow → *Search in a supernet*

AutoML



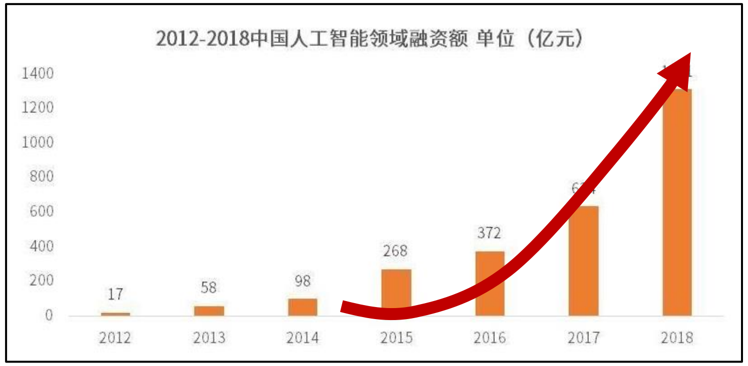
What is AutoML – Practical Viewpoint



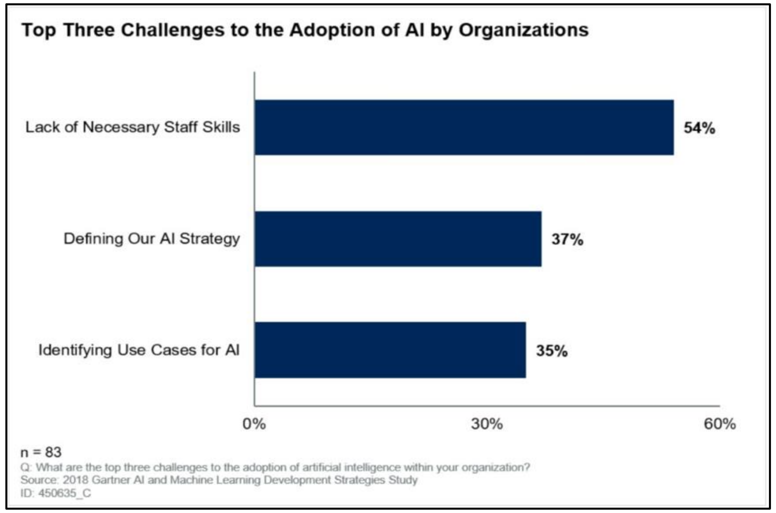
Parameterize (low-level) prior knowledge in the usage and design of machine learning

As a consequence
- Human participations can be naturally replaced by computation power
- total error of machine learning can be reduced (generalization can be improved)

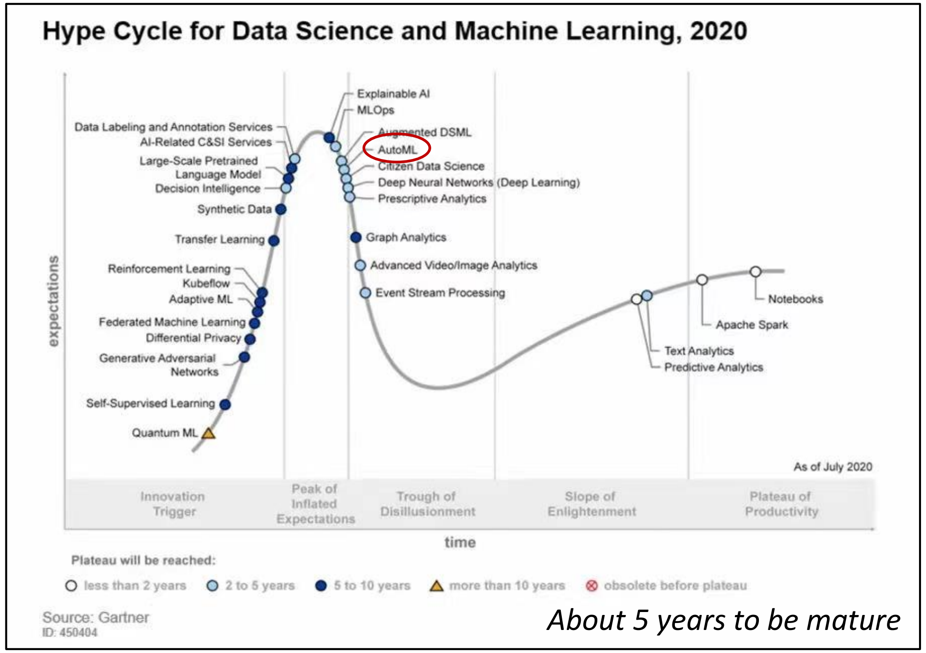
Why We need AutoML?



Investment in AI industry



Practical needs



Technical trends

- **Industry** – reduce the expense, increase usage coverage – huge market value [1]
- **Academy** – understanding data science on a higher level – great intelligence value [2,3]

[1]. Gartner: https://www.forbes.com/sites/janakirammsv/2020/03/02/key-takeaways-from-the-gartner-magic-quadrant-for-ai-developer-services/#a95b99ee3e5e
[2]. Y. Bengio: From System 1 Deep Learning to System 2 Deep Learning | NeurIPS 2019
[3]. F Hutter, L Kotthoff, J Vanschoren. Automated machine learning: methods, systems, challenges. Book 2019

Outline

1. What is Machine Learning?
2. What is Automated Machine Learning (AutoML)?
   - Explanation from a Simple Example
   - Recent Industrial and Research Examples
   - A Generalization Viewpoint for AutoML
   - How to use AutoML
3. Summary & Next Works

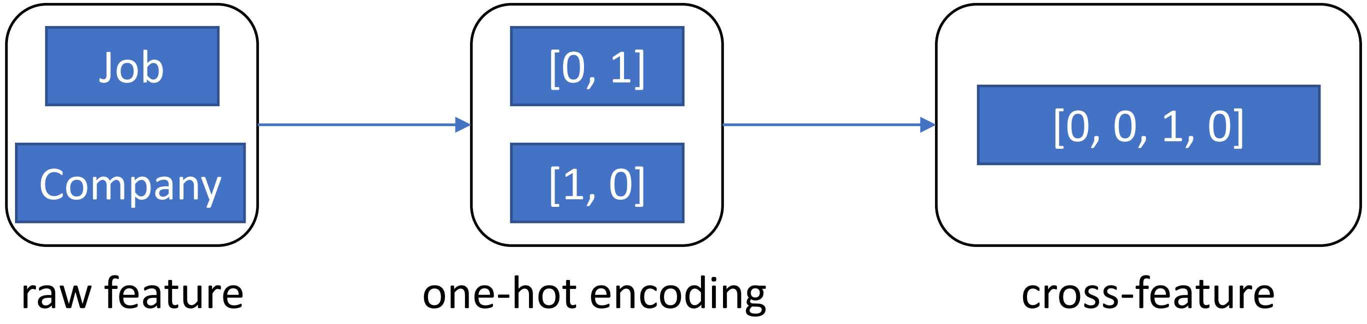
Industrial Example – Cross features

An example of tabular data (UCI-Bank)

	age (n)	job (c)	marital (c)	education (c)	balance (n)	housing (c)
0	30	unemployed	married	primary	1787	no
1	33	services	married	secondary	4789	yes
2	35	management	single	tertiary	1350	yes
3	30	management	married	tertiary	1476	yes
4	59	blue-collar	married	secondary	0	yes
5	35	management	single	tertiary	747	no

- Use one-hot/multi-hot encoding for categorical features
- Cross-features are empirically effective to enhance categorical features

Cross feature ‘job x company’ indicates that an individual takes a specific job in a specific company, and is a strong feature to predict one’s income



Not all cross-features are useful and too many of them lead to overfitting

How to find them?

[1]. Y. Luo, et.al. AutoCross: Automatic Feature Crossing for Tabular Data in Real-World Applications. KDD 2019

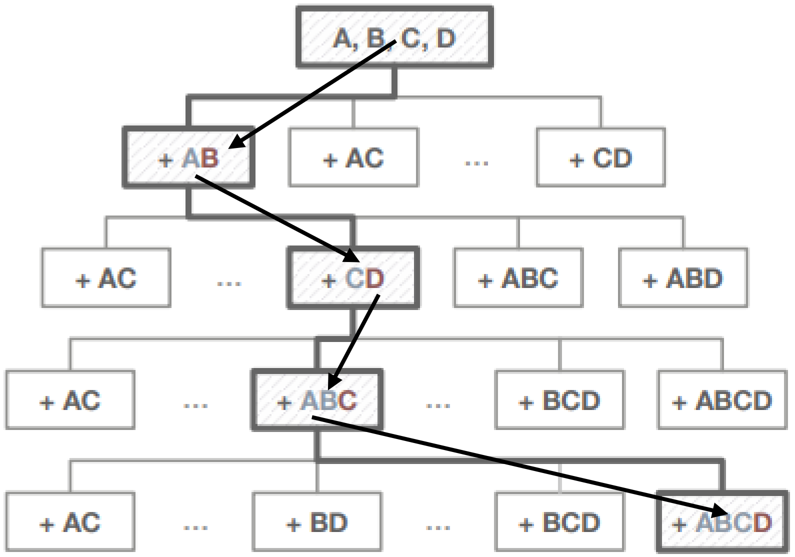
Industrial Example – AutoCross

Search cross features by bi-level optimization

$$\max_{\mathcal{S}\subseteq\mathcal{A}(\mathcal{F})} \underbrace{\mathcal{E}(\overbrace{\mathcal{L}(\mathcal{D}_{tr},\mathcal{S})}^{1},\mathcal{D}_{vld},\mathcal{S})}_{2},$$

1. Obtain a classifier on training set with current cross-feature candidates
2. Measure cross-features' performance on validation set

All possible candidates

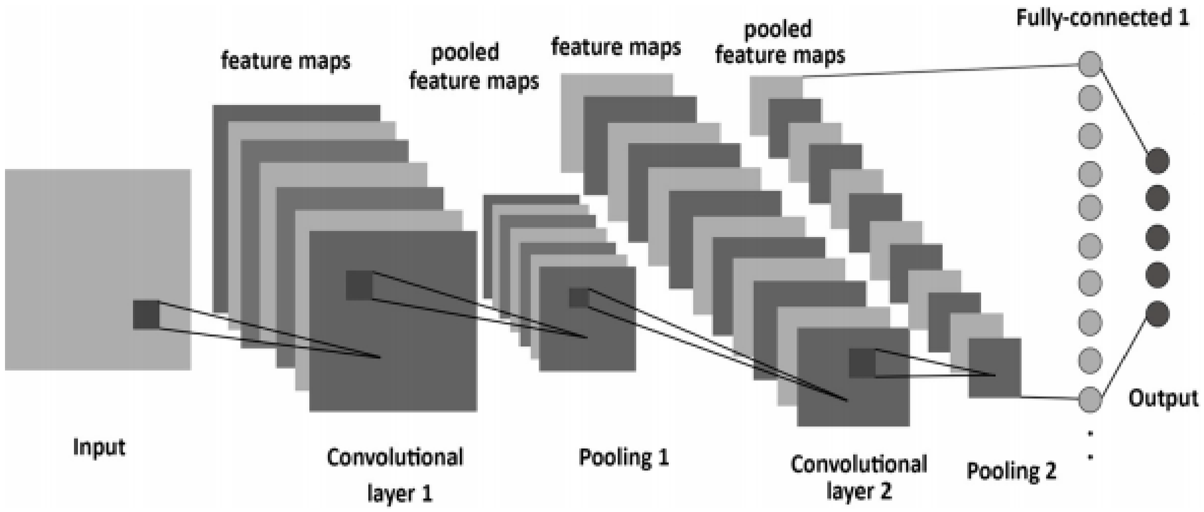


Candidate search process

[1]. Y. Luo, et.al. AutoCross: Automatic Feature Crossing for Tabular Data in Real-World Applications. KDD 2019

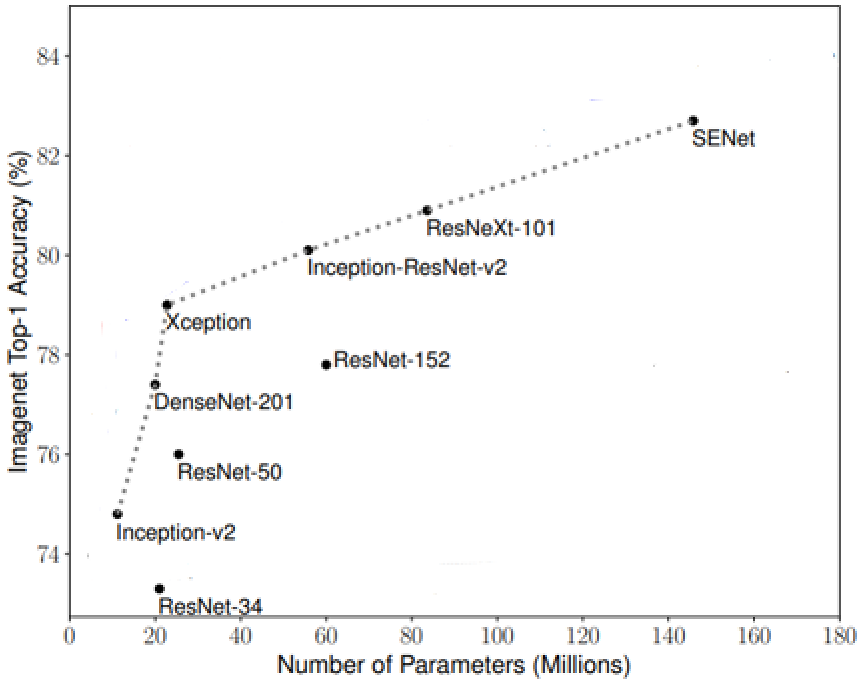
Industrial Example – AutoCross

Academic Example – Neural archi. search (NAS)



Design choice in each layer

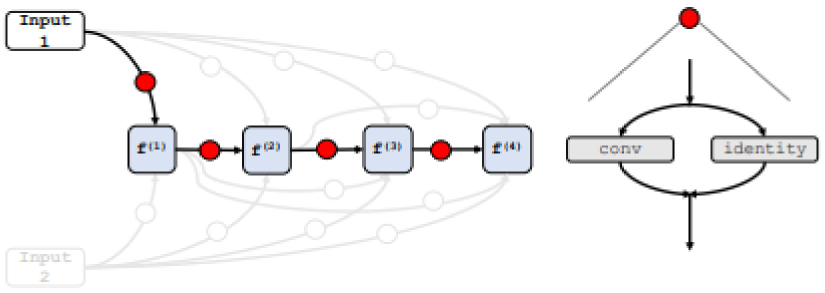
- number of filters
- filter height
- filter width
- stride height
- stride width
- skip connections



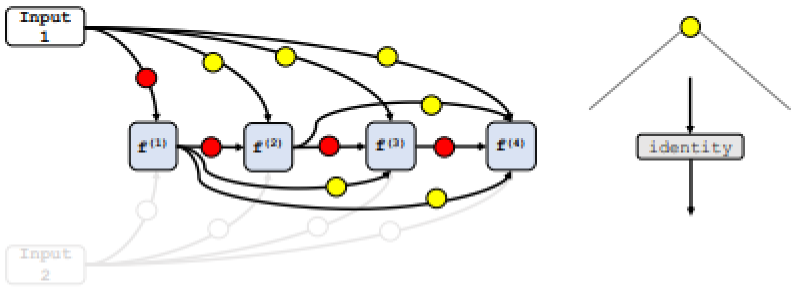
The design of architectures is important to CNN performance

Right figure: EfficientNet: Rethinking Model Scaling for Convolutional Neural Networks. ICML 2019
Left figure: Gradient-based learning applied to document recognition. 1998

NAS – Search problem

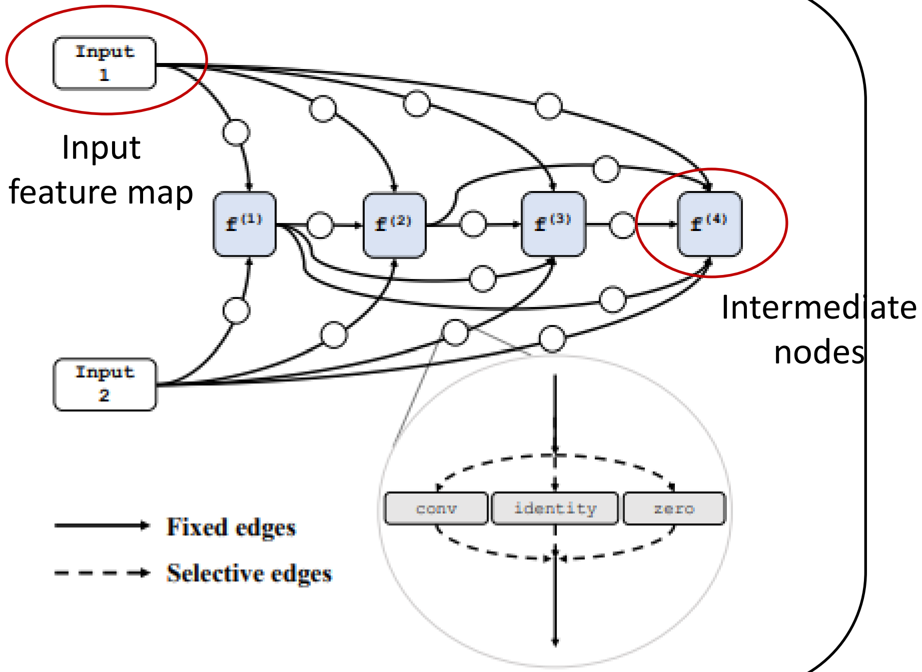


ResNet



DenseNet

Special cases

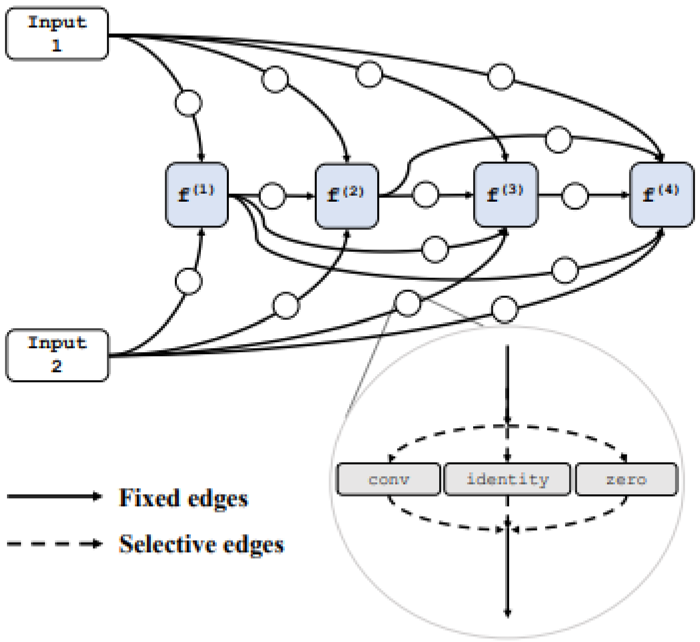


Example search space

- All possible candidates form a big supernet
- An architecture is a sub-graph in the supernet

Figures is from. M. Guo et.al. When NAS Meets Robustness: In Search of Robust Architectures against Adversarial Attacks. CVPR 2020

NAS – Search problem



Bi-level objective:

$$\min_{\mathbf{A}} \ \mathcal{F}\left(w^*, \mathbf{A}\right), \text{s.t.} \begin{cases} w^* = \arg\min_{w} \mathcal{L}_{\text{train}}\left(w, \mathbf{A}\right) \\ \mathbf{a}^{(i,j)} \in \mathcal{C} \end{cases}$$

- Train the selected architecture (encoding by $\mathbf{A}$) on training set
- Obtain the generalization performance of $\mathbf{A}$ on validation set

Typical search algorithms

- One-shot method[1,2] (fast but not accurate)
  - Alternative update architecture parameter $\mathbf{A}$ and network weights w^* by epochs
- Stand-alone method[3,4] (accurate but slow)
  - Obtain w^* by train network from scratch with given $\mathbf{A}$

[1]. H. Liu et al. Darts: Differentiable architecture search. ICLR 2018
[2]. A. Zela et al. Understanding and robustifying differentiable architecture search. ICLR 2020
[3]. Neural Architecture Search with Reinforcement Learning. ICLR 2017
[4]. K. Eggensperger. Et al. Efficient Benchmarking of Algorithm Configurators via Model-Based Surrogates. ML 2018

NAS – Promising performance

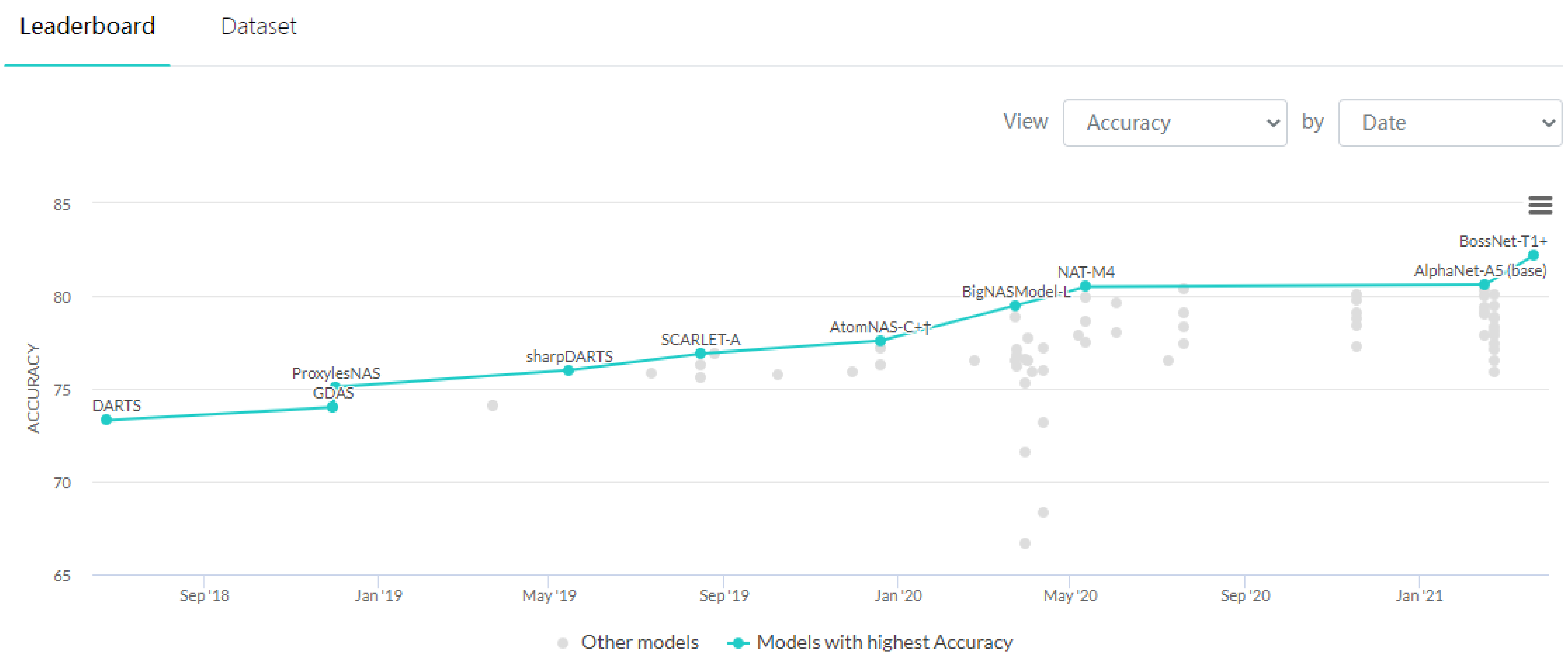


Figure is from: https://paperswithcode.com/sota/neural-architecture-search-on-imagenet

IJCAI 2021 MONTREAL

Outline

1. What is Machine Learning?
2. What is Automated Machine Learning (AutoML)?
    - Explanation from a Simple Example
    - Recent Industrial and Research Examples
    - A Generalization Viewpoint for AutoML
    - How to use AutoML
3. Summary & Next Works

Figure 4.1 & 4.2. M. Mohri, A. Rostamizadeh, A. Talwalkar. Foundations of machine learning. 2018
[1]. P. Battaglia. et.al. Relational inductive biases, deep learning, and graph networks. arXiv 2018.

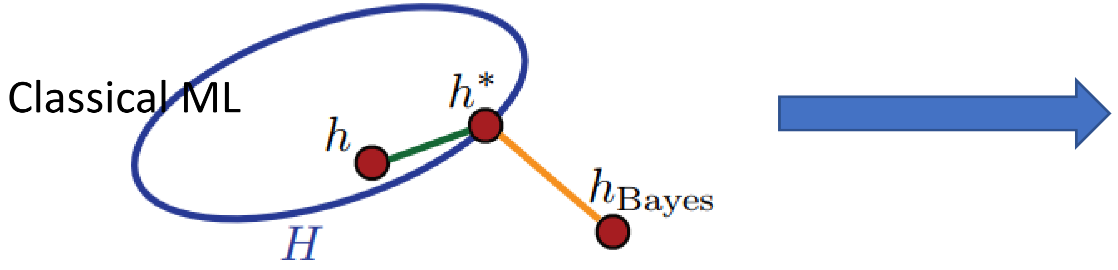
What is AutoML – Generalization viewpoint

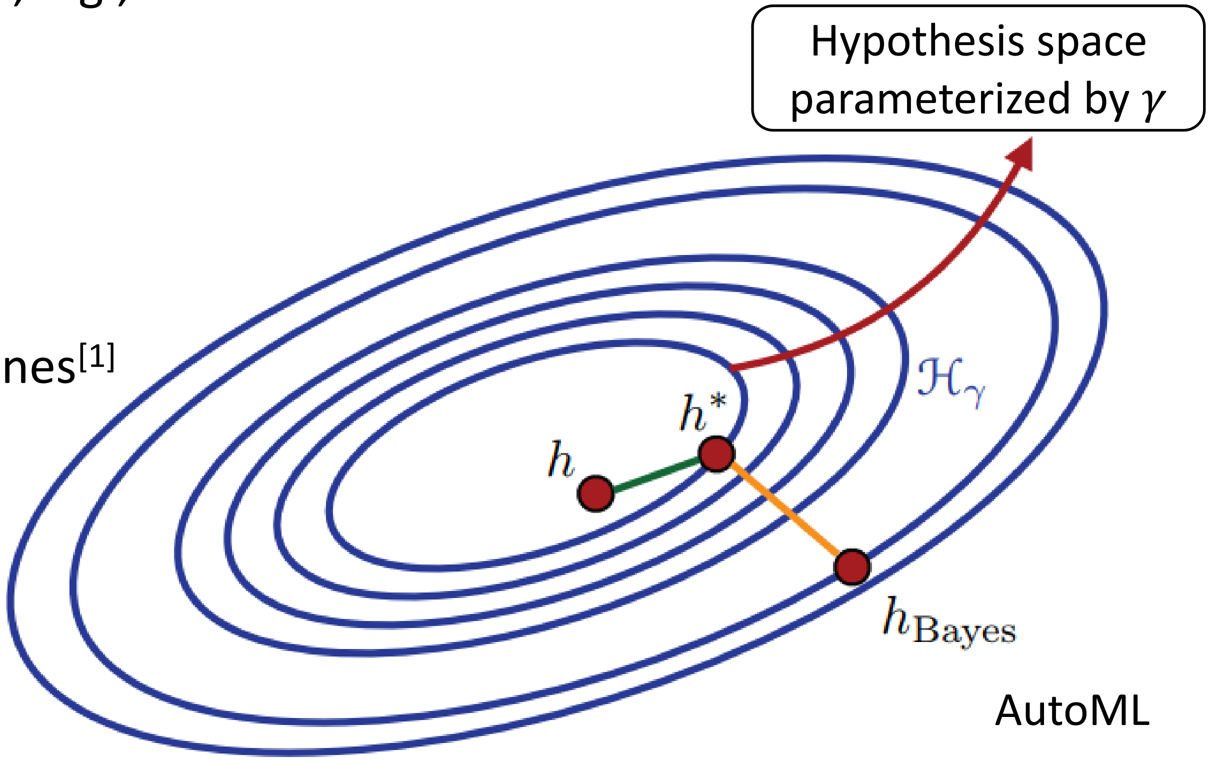
Parameterized the prior knowledge of learning methods, e.g.,

- minimize the total error
- reduce parameter numbers

Perform efficient search in the designed (new) space

- combinatorial generalize new models from existing ones[1]





Parameterize (low-level) prior knowledge in the usage and design of machine learning

As a consequence
- Human participations can be naturally replaced by computation power
- total error of machine learning can be reduced (generalization can be improved)

AutoML – Successor of ML's trend

- Core Issue in Machine Learning: Improving learning performance (with higher efficiency)
- AutoML: an evolving way to improve learning performance

Rule-based
1990s

Statistics-based
2000s

Deep Learning-based
2010s

AutoML-based
From 2017

Continue the trends

- Larger hypothesis (more complex models) are being used
- Optimization is getting complex (even mixed up with generalization)
- The prior knowledge is imposed on more abstract level

Better performance

Parameterize (low-level) prior knowledge in the usage and design of machine learning

Related Areas

Sub-areas

- Neural architecture search
- Hyper-parameter search
- Automated feature engineering
- Algorithms selection
- Model selection

Related areas

- Bi-level / Derivative-free optimization
  - Focus more on algorithm design
  - AutoML objective is one kind of objective where these algorithms can be applied
- Meta-learning
  - Focus on parameterize task distributions
  - Another kind of bi-level objective
  - Do not use validation set to update hyper-parameters

Outline

1. What is Machine Learning?
2. What is Automated Machine Learning (AutoML)?
   - Explanation from a Simple Example
   - Recent Industrial and Research Examples
   - A Generalization Viewpoint for AutoML
   - How to use AutoML
3. Summary & Next Works

How to use AutoML

1. Define an AutoML problem

- Derive a search space from insights in specific domains
- Search objective is usually validation performance
- Search constraint is usually resource budgets
- Training objective usually comes from classical learning models

$$\min_{\boxed{\lambda\in\mathcal{S}}} \boxed{M(F(w^*;\lambda), D_{\text{val}})}$$

Search Space

Search Objective

$$\text{s.t.} \begin{cases} \boxed{\min_{w} L(F(w;\lambda), D_{\text{tra}})} \\ \boxed{G(\lambda) \leq C} \end{cases}$$

Training Objective

Search Constraints

2. Design or select proper search algorithm

- Reduce model training cost (time to get w^*)

What is AutoML – Short summary

- Exploring prior knowledge is important in machine learning
  - Cost time and critical to generalization performance
  - Continual trends in ML: imposing the prior knowledge on more abstract level
- AutoML attempts to parameterize low-level prior knowledge
  - Human participations can be naturally replaced by computation power
  - total error can be reduced (generalization can be improved)
- To use well AutoML techniques
  - Exploring high-level domain knowledge when defining the AutoML problem
  - Reducing model training cost when design search algorithm

Outline

1. What is Machine Learning?
2. What is Automated Machine Learning (AutoML)?
3. Summary & Next Works

Summary & Next Works

1. An introduction to Automated Machine Learning (AutoML)
   - Background on technical tools from machine learning
2. Why AutoML is Needed in RecSys and Recent Advances
   - Exemplar works introducing AutoML into RecSys
3. Automated Graph Representation Learning for RecSys
   - Explore neural architecture search for GNN based RecSys
4. Automated Knowledge Graph (KG) Embedding
   - Explore AutoML for KG Embedding based RecSys

Thanks!