AutoML - MVA 2020-2021





# Automated Machine Learning

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# AutoML: an intro

# Successes of Machine learning



Computer vision



Games



... relies on **extensive** and **manual** tuning of algorithms and their hyperparameters



## Machine Learning

#### Machine Learning algorithm: Decision Tree, CNN, SVM, etc

Dogs vs Cats dataset



 $P(\alpha_{\theta})$ 

performance (e.g. accuracy)

IN (for another A)

nother A)

encoded by: hyperparameters  $\lambda \in \Lambda$ hand-crafted by <u>ML experts</u>



## The AutoML problem: definition



 $(D_{tr}, \beta_1, \alpha_1, P_1), (D_{tr}, \beta_2, \alpha_2, P_2), (D_{tr}, \beta_3, \alpha_3, P_3), \dots$ 

Table 7.1 Supervised learning illustration of the three-level formulation. An algorithm's level is entirely determined by its type of *input* and *output*. For a given task, finding a good  $\alpha$ -level algorithm is the ultimate goal.  $\gamma$ -level algorithms exploit data from *all past experience*, in the form of a "meta-dataset", to allow us to select a better  $\beta$ -level algorithm, which in turn exploits the dataset of a given task to produce an  $\alpha$ -level algorithm by training.

Level	Input	Output	Examples	Encoded by
α-	sample or	prediction	heuristically hard-	parameters,
level	example	of label	coded classifier	hyper-parameters
	(e.g. an	(e.g. 'dog'	or already trained	(if any) and
	image)	or 'cat')	classifier	meta-parameters
				(if any)
β-	task/dataset	$\alpha$ -level al-	learning algorithms	hyper-parameters
level	(e.g.	gorithm	(e.g. SVM, CNN);	and meta-
	MNIST,		HPO algorithms	parameters
	CIFAR-		(e.g. grid search	(if any)
	10)		cross-validation,	
			SMAC [56],	
			NAS [124])	
γ-	meta-	$\beta$ -level al-	meta-learning algo-	meta-parameters
level	dataset (e.g.	gorithm	rithms (e.g. meta-	
	OpenML		learning part in	
	[115])		Auto-sklearn [36]);	
			algorithms from this	
			thesis.	

# AutoML: what's exciting?

- 100% autonomous
- Beat "no free lunch"
- Any time
- Any resource





# AutoML: a trending topic



Google's AutoML









Traditional Machine Learning Workflow



AutoML Workflow





# AutoML methods with application to Deep Learning

We'll focus on the simplest case

 $\mathfrak{D}_{tr} = \emptyset$  (initially) and  $\mathfrak{D}_{te} = \{(D_{tr}, D_{te})\}$  (single dataset)

Hyperparameter Optimization

 $\longrightarrow$  single fixed training dataset:  $D_{tr}$ 

we only need to focus on  $\beta_{\lambda}, \lambda \in \Lambda$ 

#### Reminder:

$$\max_{\gamma} \sum_{\substack{D_{tr}, D_{te} \\ \in \mathfrak{D}_{te}}} P(\hat{\hat{\alpha}}; D_{te}) \qquad \text{where } \hat{\hat{\alpha}} = \hat{\beta}(D_{tr}) \text{ and } \hat{\beta} = \gamma(\mathfrak{D}_{tr})$$

#### Hyperparameter Optimization: a reformulation

an HPO algorithm aims to solve:  $\max_{\lambda \in \Lambda} P(\hat{\alpha}; D_{te})$  where  $\hat{\alpha} = \beta_{\lambda}(D_{tr})$ 

unknown test score:  $P(\hat{\alpha}; D_{te}) \implies$  use an estimation (e.g. CV):  $\hat{P}(\lambda)$ 

so usually the problem becomes



 $\hat{P}: \Lambda \to \mathbb{R}$ 

black-box optimization

expensive to compute

where

surrogate model (not discussed)

$$\lambda \mapsto s = \hat{P}(\lambda) \approx P(\beta_{\lambda}(D_{tr}), D_{va})$$

is an estimation of the test score

Remark: some approaches optimize  $\lambda$  and  $\theta$  at the same time

bi-level optimization (ex. DARTS H. Liu et al., 2018)

#### $\beta_{\lambda}, \lambda \in \Lambda$ encodes an architecture A



Image adapted from: Automated Machine Learning - Methods, Systems, Challenges, Frank Hutter et. al, (2018) Springer.

- 3 ingredients in HPO (NAS):
- Search space
- Search strategy
- Performance estimation strategy

# Search Space (for DL)

 $\beta_{\boldsymbol{\lambda}}, \boldsymbol{\lambda} \in \boldsymbol{\Lambda} \,:$  architecture, optimizer, regularization, etc



Different layer types are visualized by different colors.

Automated Machine Learning - Methods, Systems, Challenges, Frank Hutter et. al, (2018) Springer.

# Search Space (for DL)



#### "NASNet search space" only uses two building blocks

Zoph B, Vasudevan V, Shlens J, Le QV. Learning Transferable Architectures for Scalable Image Recognition. CVPR2018

Softmax



 $\Lambda = \Lambda_1 \times \Lambda_2$  with  $\Lambda_1 = \{1, 2, 3, 4\}$  and  $\Lambda_2 = \{0.001, 0.001, 0.1, 1\}$ 

# neurons in hidden layer

learning rate

try every possible combination in

$$\Lambda = \Lambda_1 \times \Lambda_2$$

evaluate it and return argmax in the end

curse of dimensionality!



## Random Search

$$\Lambda = \Lambda_1 \times \Lambda_2$$
 with  $\Lambda_1 = \{1, 2, 3, 4\}$  and  $\Lambda_2 = \{0.001, 0.001, 0.1, 1\}$ 

*#* neurons in hidden layer

learning rate

Randomly sample certain number of combinations in

$$\Lambda = \Lambda_1 \times \Lambda_2$$

evaluate it and return argmax in the end



## Grid Search and Random Search

two model-free black-box optimization methods



RS tends to perform better than GS when some HP are more important than others Random Search provides already a strong HPO baseline (surprisingly...?)

Bergstra J, Bengio Y. Random Search for Hyper-Parameter Optimization. JMLR. 2012

# **Evolutionary Algorithms**

Population-based derivative-free optimization methods



similar to: genetic algorithms, evolutionary strategies, particle swarm optimization

Optimize w.r.t a population (a set of points) or a distribution instead of one single point

Often encode an individual by "chromosome"

Explore new points by mutation or crossover

Select individuals by fitness

Just some vocabulary...but the idea is simple

Easy to parallelize

## Evolutionary Algorithm: an example

Real E, Moore S, Selle A, et al. Large-Scale Evolution of Image Classifiers. ICML2017

1000 individuals

fitness: accuracy on validation dataset

pair-wise competition (select two individuals and kill the weaker one)

the winner gets to reproduce and mutate

massively-parallel (due to huge computation cost)

chromosome (DNA): tensor graph

begins from single layer individuals

possible mutations:

- ALTER-LEARNING-RATE
- IDENTITY
- RESET-WEIGHTS
- INSERT-CONVOLUTION
- REMOVE-CONVOLUTION.
- ALTER-STRIDE
- ALTER-NUMBER-OF-CHANNELS
- FILTER-SIZE
- INSERT-ONE-TO-ONE
- ADD-SKIP
- REMOVE-SKIP

## Evolutionary Algorithm: an example



Real E, Moore S, Selle A, et al. Large-Scale Evolution of Image Classifiers. ICML2017

## **Bayesian Optimization**

$$\max_{\lambda \in \Lambda} \hat{P}(\lambda) \quad \text{with } \hat{P} : \Lambda \to \mathbb{R} \\ \lambda \mapsto s$$

Original idea:  $\lambda$  and  $s = \hat{P}(\lambda)$  follow prior distributions  $p(\lambda), p(s | \lambda)$ 

we choose next point to evaluate by maximizing an acquisition function (active learning-like)

we gain more information and update  $p(\lambda)$  and  $p(s|\lambda)$  (or  $p(s,\lambda)$ )

repeat until convergence



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# Bayesian Optimization (cont'd)

$$\max_{\lambda \in \Lambda} \hat{P}(\lambda) \quad \text{with } \hat{P} : \Lambda \to \mathbb{R} \\ \lambda \mapsto s$$

usual acquisition function: Expected Improvement (EI)

 $a_{EI}(\lambda | D_n) = \mathbb{E}[\max(\hat{P}(\lambda) - s_{\max}, 0)]$ 

usual prior model: Gaussian Process (GP)

but state-of-the-art tends to use tree-based classifier such as **Random Forest** to model

 $\hat{P}(\lambda)$  (or  $p(s \,|\, \lambda)$  )

(thus not so Bayesian anymore...), see Auto-sklearn



### Bayesian Optimization: an example

Swersky K, Snoek J, Ada;s RP. Freeze-Thaw Bayesian Optimization. 2014

Intuition:

Maintains a set of "frozen" (partially completed but not being actively trained) models and uses an information-theoretic criterion to determine which ones to "thaw" and continue training

Use Bayesian Optimization for:

- learning curve prediction -> offers quick evaluations
- HP space modeling



use notation  $f: x \mapsto y$  instead of  $\hat{P}: \lambda \mapsto s$ 

## **Reinforcement Learning**

A reminder:



State space: STransition model:  $\mathscr{P}^{a}_{ss'} = p(s'|s, a) : S \times A \times S \rightarrow [0,1]$ Action space: AReward:  $\mathscr{R}^{a}_{ss'} : S \times A \times S \rightarrow \mathbb{R}$ 

**Goal:** Learn a policy:  $\pi(s, a) = p(a | s) : S \times A \rightarrow [0, 1]$ 

that maximizes the (discounted) expected return

$$\mathbb{E}_{\pi}\left[\sum_{t=1}^{T}\gamma^{t}r_{t}\right]$$

with  $T \in [0, +\infty], \gamma \in [0,1]$  and  $s_0, a_0, r_1, s_1, a_1, r_2, s_2, a_2, ...$  the agent's trajectory

## Reinforcement Learning: an example

Zoph B, Le QV. Neural Architecture Search with Reinforcement Learning. ICLR 2017



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# Summary

Method	Туре	How to take next action	Update/Learn			
Grid Search	model-free	loop over all choices (Cartesian product)	take max			
Random Search	model-free	totally random	take max			
Bayesian Optimization	sequential-based	maximizes acquisition function	update surrogate model			
Evolutionary Algorithms	population-based	each individual randomly mutates	eliminate the weakest (with least fitness)			
Reinforcement Learning	mixed/can be very general	according to learned policy	policy gradient method			
Differentiable Methods	gradient-based	follow (negative) gradient	gradient descent			
There is learning in EVERY method						
Is there exploration-exploitation trade-off in each method?						
How do we do benchmarking and fairly evaluate these methods?						
Autopl challenge!!!						

## Some other AutoML methods

**Transfer Learning** 

Meta-learning

Ensemble methods (competition winners)

embedded methods\*: bi-level optimization methods (related to transfer learning)

filter methods\*: narrowing down the model space, without training the learning machine (related to meta-learning)

\* Guyon I, Bennett K, Cawley G, et al. Design of the 2015 ChaLearn AutoML challenge. IJCNN 2015

## From one to multiple datasets: meta-learning

Given:

- Algorithms  $j = 1, \ldots, m$
- ▶ PAST datasets i = 1, ..., n 1
- a NEW dataset n

**Meta-dataset**: S where S(i, j) = score of algo. j applied on dataset i.

Find

 $\operatorname{argmax}_{j=1,\dots,m} \mathbf{S}(n,j)$ 

I.e. We want to learn some transferable knowledge across datasets (a meta-learning model  $\gamma$ ), to solve a new dataset better and faster.

### Meta-Learning: 1st trial with Auto-sklearn

Feurer M, Klein A, Eggensperger K, Springenberg JT, Blum M, Hutter F. Efficient and Robust Automated Machine Learning. 2015

#### Intuition: Warm start the BO with meta-learning techniques, ensemble the top models.



Figure 1: Our improved approach to AutoML. We add two components to Bayesian hyperparameter optimization of an ML framework: meta-learning for initializing the Bayesian optimizer and automated ensemble construction from configurations evaluated during optimization.

#### Meta-learning [Brazdil et al., 2009]:

- characterize the dataset using meta-features,
- Initialize BP with config. That performed well on old similar dataset

#### **BO subroutine:** SMAC [Hutter et al. 2011]:

- Random Forest prior
- Expected improvement acquisition
- 1 fold quick evaluation

### Meta-Learning: example 2

## Model-Agnostic Meta-Learning [Finn et al. 2017]

- Assumption: a single learning algorithm (NN)
- Setting: Given a distribution of datasets noted D; with ω<sub>i</sub> the optimal model for D<sub>i</sub>

MAML finds a generally good solution:

$$\boldsymbol{\omega} = \operatorname{argmax} \sum_{D_i} s_{D_i} (\boldsymbol{\omega} - \alpha \nabla_{\boldsymbol{\omega}} s_{D_i})$$

This solution is used as starting point for the new pb.



# AutoML challenges

### The AutoML challenge (Guyon et al., 2015-2016)



image

medical

speech

marketing

#### Task variabilities:

- classification / regression
- various scoring functions
- various time budget
- etc.

#### Goal: Find a process to identify the best $\beta_{\lambda}$ for each task

[1]: Design of the 2015 ChaLearn AutoML challenge, Guyon et al., 2015

[2]: Lessons learned from the AutoML challenge, Sun-Hosoya, Guyon and Sebag, 2018

## After the AutoML challenge series

http://automl.chalearn.org/



#### AutoDL https://autodl.chalearn.org/



NumberofEpochs ConvolutionKernelWidth Optimiser Regularization BatchNormalization ActivationFunction WeightDecay NetworkWeightInitialization DropoutMiniBatchSize Momentum NumberofHiddenLayers LearningRate

# AutoDL challenge 2019-2020



• IMAGE

- VIDEO
- SPEECH
- TEXT
- TABULAR
- Multi-label tasks

Liu Z, Xu Z, Rajaa S, Madadi M. Towards Automated Deep Learning: Analysis of the AutoDL challenge series 2019. To appear in *NeurIPSCD2019* in Proceedings of Machine Learning Research (PMLR) 2019:10.

- (1) Raw data from 5 modalities: Image, Video, Speech, Text, Tabular.
- (2) Fixed time budget. Any-time learning (ALC metric). Blind testing.
- (3) Starting kit, sample "public" data and baselines provided.
- (4) Fixed computational resources.
- (5) Using Deep Learning was NOT imposed.

#### Neural architectures used in the winning approaches



Architecture name	# Parameters	Domains	Teams
ResNet-18, ResNet-9 ( <u>He et al</u> 2015)	11.4M, 5.7M	image, video	Kakaobrain, DeepWisdom, automl_freiburg
MC3 ( <u>Du Tran et al CVPR 2018</u> )	32.8M	video	DeepWisdom
EfficientNet-(b0, b1, b2) ( <u>M. Tan and Q. Le. 2019</u> )	5.3M, 7.8M, 9.2M	image, video	DeepWisdom, automl_freiburg
MobileNetV2 ( <u>M. Sandler et al</u> 2019)	3.4M	image, video	team_zhaw, DeepBlueAl
TextCNN	variable	text	Upwind_flys, DeepWisdom
Fast RCNN (Ross Girshick)		text	DeepWisdom
LSTM, BiLSTM ( <u>Hochreiter,</u> <u>Schmidhuber 1997</u> )	0.2M-1M	text, speech	frozenmad, PASA_NJU
GRU, BiGRU, ( <u>Kyunghyun Cho et</u> <u>al 2014</u> ) GRU with Attention	0.1M-1M	text, speech	DeepBlueAl, DeepWisdom
BERT-like (Tiny-BERT( <u>X.Jiao</u> et al))	<110M	text	frozenmad, upwind_flys
DNN	<1M	tabular	DeepWisdom

#### AutoML techniques vs domains

Approach	image	video	speech	text	tabular
Meta-learning	Offline meta-training transf	erred with AutoFolio [25] ba	ased on meta-features (aut	oml freiburg)	•
	Offline meta-training gener	rating solution agents, sear	ching for optimal sub-opera	tors in predefined sub-spa	ces, based on dataset
	meta-data. (DeepWisdom)				
	IVIAIVIL-IIKe method [17] (te	am znaw)	MECC Mal Speatrogram	Iroot tooturoo ovtrootiono	Numerical and
Preprocessing	( <i>PASANJU</i> ), fast	frames and adaptive image size (DeepBlueAI)	STFT	with stemmer, meaningless words	Categorical data detection and encoding
	(DeepBlueAl)	Adaptive image size		Intering (DeepBlueAI)	
Hyperparameter Optimization	Offline with BOHB [26] (Ba Model-Based Optimization	yesian Optimization and M for General Algorithm Con	ulti-armed Bandit) ( <i>automl</i> figuration (SMAC) ( <i>automl</i>	freiburg) Sequential freiburg)	Baysien Optimization ( <i>PASANJU</i> ) HyperOpt [27] ( <i>Inspur AutoDL</i> )
Transfer learning	Pre-trained on ImageNet	Pre-trained on ImageNet	ThinResnet34 pre-trained	FastText pre-trained on	
	Kon)	except Kon) MC3 model	(DeepWisdom)	Common Crawl	
		(DeepWisdom)		(frozenmad)	
Ensemble	Adaptive Ensemble	Ensemble Selection [29]	last best predictions	Weighted Ensemble over	LightGBM ensemble with
learning	Learning (ensemble latest 2 to 5 predictions) (DeepBlueAI)	(top 5 validation predictions are fused) (DeepBlueAI): Ensemble	(DeepWisdom) averaging 5 best overall and best of	(DeepWisdom)	Dagging method [30] (DeepBlueAl), Stacking and blending
		models sampling 3, 10, 12 frames (DeepBlueA)	each model: LR, CNN, CNN+GRU ( <i>DeepBlueA</i> )		(DeepWisdom)

leams	VC	don	າລເກດ
ICams	٧J	uon	I an I o

leam	image	video	speech	text	tabular
DeepWisdom	[ <b>ResNet-18</b> and ResNet-9 models] [pretrained on ImageNet]	[MC3 model] [pretrained on Kinetics]	[fewshot learning ] [LR, ThinRestnet34 models] [pretrained on VoxCeleb2]	[fewshot learning] [task difficulty and similarity evaluation for model selection] [SVM, TextCNN [fewshot learning] RCNN, GRU, GRU with Attention]	[LightGBM, Xgboost, Catboost, DNN models] [no pretrained]
DeepBlueAl	[data augmentation with Fast AutoAugment] [ResNet-18 model]	[subsampling keeping 1/6 frames] [Fusion of 2 best models ]	[iterative data loader (7, 28, 66, 90%)] [MFCC and Mel Spectrogram preprocessing] [LR, CNN, CNN+GRU models]	[Samples truncation and meaningless words filtering] [Fasttext, TextCNN, BiGRU models] [Ensemble with restrictive linear model]	[3 LightGBM models] [Ensemble with Bagging]
PASANJU	ResNet-18 and SeResnext50; preprocessing: shape standardization and image flip (data augmentation)	ResNet-18 and SeResnext50; preprocessing: shape standardization and image flip (data augmentation)	[data truncation(2.5s to 22.5s)][LSTM, VggVox ResNet with pretrained weights of DeepWis- dom(AutoSpeech2019) ThinRestnet34?]	[data truncation(300 to 1600 words)][TF-IDF and word embedding]	[iterative data loading] [Non Neural Nets models] [models complexity increasing over time] [Baysien Optimization of hyperparameters]
frozenmad	Images resized under 128x128] [progressive data loading increasing over time and epochs] [ResNet-18 model] [pretrained on ImageNet]	[Successive frames difference as input of the model] [pretrained <b>ResNet-18</b> with RNN models]	[progressive data loading in 3 steps 0.01, 0.4, 0.7] [time length adjustment with repeating and clipping] [STFT and Mel Spectrogram preprocessing] [LR, LightGBM, VggVox models]	[TF-IDF and BERT tokenizers] [ SVM, RandomForest , CNN, tinyBERT ]	[progressive data loading] [no preprocessing] [Vanilla Decision Tree, RandomForest, Gradient Boosting models applied sequentially over time]

#### Lessons learned from the AutoDL challenge

- (1) The winning methods are capable of generalizing on new unseen datasets => Potential universal AutoML solutions
- (2) Domain-dependent approaches are dominant
  => No universal workflows, mostly hand-tuned meta-learning
- (3) We cannot afford to run expensive NAS for every new task
  => Need transferability of learned architectures
- (4) Beating Baseline 3 by using "true" meta-learning is hard
  => Need more meta-train datasets (public datasets)

# MetaDL challenge

	Input	Output	Comp. Ex.
Alpha level: predict() in sklearn, a classifier	X example/sample (e.g. an image)	У labels	Code Jam LeetCode
Beta level: fit() in sklearn, a learning algo.	T ML task (dataset)	$oldsymbol{lpha}$ alpha-level algo	(Auto)ML challenges & AutoDL
Gamma level: meta_fit() on a meta-dataset	D Meta-dataset	$oldsymbol{eta}$ beta-level algo	MetaDL

Check and stay tuned <a href="https://metalearning.chalearn.org/">https://metalearning.chalearn.org/</a>

# Conclusion

## Take-home messages

AutoML problem can be formulated in 3 levels:  $\alpha \leftarrow \beta \leftarrow \gamma$ 

Domain specific AutoML solution generalizes

Hand-crafted gamma-level learning => Cross-domain meta-learning yet to be studied

Any-time learning aspect to be studied further

## Stay tuned! autodl.chalearn.org

