Deep Learning in Practice - MVA 2019-2020





Automated Deep Learning

LIU Zhengying

Laboratoire en Recherche Informatique (LRI) U. Paris-Sud / Inria / U. Paris Saclay

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Contents

• AutoML: an intro

• AutoML methods with application to Deep Learning

AutoDL challenges

AutoML: an intro





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 typical process...



Normal spirals





zero hyperparameters no hand-crafting at all! actually defines a beta: $\beta_{\pi}(D) := \pi(D)(D)$ can be learned too \implies meta-learning



can be combined with Hyperparameter Optimization we can also have $\mathfrak{D} = \{D_j, \beta_j, \alpha_j, P_j\}$ with trained $\alpha_j \implies$ transfer learning



The AutoML problem: definition



Exercise: a toy example



neural network with one hidden layer $\theta? \ \lambda?$ hard-coding approach? ML? AutoML?

AutoML: what's exciting?

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





AutoML: already a hot 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:

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

Search Space

How do we describe (encode) a learning algorithm?



in <u>natural language</u>:

"a feed-forward neural network with one hidden layer of p=10 neurons, using ReLU as activation and Adam as optimizer, with learning rate lr=0.001, ..."

formally:

 $\beta_{\lambda}, \lambda \in \Lambda$??

Search Space (for DL)

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



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

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)

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

is an estimation of the test score

Remark: some approaches optimize λ and θ at the same time

bi-level optimization (to be discussed later with DARTS)

Search Strategy

- Heuristic search
 - Grid Search
 - Random Search
 - Evolutionary Algorithms
- Bayesian Optimization
- Reinforcement Learning methods
- Differentiable methods

 $\Lambda = \Lambda_1 \times \Lambda_2$ 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: λ 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



29

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

Bergstra JS, Bardenet R, Bengio Y, Kégl B. Algorithms for Hyper-Parameter Optimization. NIPS2011

Tree Parzen Estimator (TPE) -> Hyperopt model $p(\lambda | s < \alpha)$ and $p(\lambda | s > \alpha)$ instead of $p(s | \lambda)$ use notation $f : x \mapsto y$ instead of $\hat{P} : \lambda \mapsto s$

$$p(x|y) = \begin{cases} \ell(x) & \text{if } y < y^* \\ g(x) & \text{if } y \ge y^*, \end{cases}$$

$$\mathrm{EI}_{y^*}(x) = \int_{-\infty}^{y^*} (y^* - y) p(y|x) dy = \int_{-\infty}^{y^*} (y^* - y) \frac{p(x|y)p(y)}{p(x)} dy$$

$$EI_{y^*}(x) = \frac{\gamma y^* \ell(x) - \ell(x) \int_{-\infty}^{y^*} p(y) dy}{\gamma \ell(x) + (1 - \gamma)g(x)} \propto \left(\gamma + \frac{g(x)}{\ell(x)} (1 - \gamma)\right)^{-1}$$

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



Differentiable Methods

Liu H, Simonyan K, Yang Y. DARTS: Differentiable Architecture Search. ICLR2019

Idea: relaxation of "hard" choice of operations (convolution, max-pooling, zero) to "soft" choice (linear combination of these operations)

$$\bar{o}^{(i,j)}(x) = \sum_{o \in \mathcal{O}} \frac{\exp(\alpha_o^{(i,j)})}{\sum_{o' \in \mathcal{O}} \exp(\alpha_{o'}^{(i,j)})} o(x)$$



Differentiable Methods

Liu H, Simonyan K, Yang Y. DARTS: Differentiable Architecture Search. ICLR2019

algorithm parametrized by architecture: α weights: W



Bi-level optimization:

- 1. update W on training set
- 2. update α on validation set

$$\min_{\alpha} \quad \mathcal{L}_{val}(w^*(\alpha), \alpha)$$
s.t. $w^*(\alpha) = \operatorname{argmin}_{w} \quad \mathcal{L}_{train}(w, \alpha)$

Inner step is very expensive => approximate full training by on step:

$$\nabla_{\alpha} \mathcal{L}_{val}(w^*(\alpha), \alpha)$$

$$\approx \nabla_{\alpha} \mathcal{L}_{val}(w - \xi \nabla_w \mathcal{L}_{train}(w, \alpha), \alpha)$$

Results:

Close to state-of-the-art (SotA) on image (CIFAR10, ImageNet) but much faster SotA on language modeling (Penn Treebank, WikiText-2)

Can be considered as having one single big architecture but with different training method => Lottery Ticket Hypothesis?

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?							
AutoDL 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

AutoDL challenges



Competition track @ NeurIPS 2019

AutoDL challenges

Zhengying Liu

Inria / LRI, France - zhengying.liu@inria.fr







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AutoML challenges

the origin - 2015-2018



AutoDL challenges

Towards fully automated multi-label classification for

image, video, text, speech, tabular



AutoML challenges





New Features

compared to AutoML challenges







Any-time learning

Raw data

Large scale

What is the goal of AutoDL?

Three-level formulation of AutoML

algorithm in each level is characterized uniquely by their input and output



Z. Liu et al, "Overview and unifying conceptualization of Automated Machine Learning"

Data





15 image + **10** video + **15** speech + **15** text + **50** tabular

					Class	Sample number		· ·	Tensor dimension		
#	Dataset	Challenge	Phase	Domain	number	train	test	time	row	col	channel
1	Munster	AutoCV	public	hand-writing	10	60000	10000	1	28	28	1
2	Chucky	AutoCV	public	objects	100	48061	11939	1	32	32	3
3	Pedro	AutoCV	public	people	26	80095	19905	1	var	var	3
4	Decal	AutoCV	public	aerial	11	634	166	1	var	var	3
5	Hammer	AutoCV	public	medical	7	8050	1965	1	600	450	3
6	Ukulele	AutoCV	feedback	hand-writing	3	6979	1719	1	var	var	3
7	Caucase	AutoCV	feedback	objects	257	24518	6089	1	var	var	3
8	Beatriz	AutoCV	feedback	people	15	4406	1094	1	350	350	3
9	Saturn	AutoCV	feedback	aerial	3	324000	81000	1	28	28	4
10	Hippocrate	AutoCV	feedback	medical	2	175917	44108	1	96	96	3
11	Loukoum	AutoCV	final	hand-writing	3	27938	6939	1	var	var	3
12	Tim	AutoCV	final	objects	200	80000	20000	1	32	32	3
13	Apollon	AutoCV	final	people	100	6077	1514	1	var	var	3
14	Ideal	AutoCV	final	aerial	45	25231	6269	1	256	256	3
15	Ray	AutoCV	final	medical	7	4492	1114	1	976	976	3
16	Kraut	AutoCV2	public	action	4	1528	863	var	120	160	1
17	Katze	AutoCV2	public	action	6	1528	863	var	120	160	1
18	Kreatur	AutoCV2	public	action	4	1528	863	var	60	80	1
19	Ideal	AutoCV2	feedback	aerial	45	25231	6269	1	256	256	3
20	Freddy	AutoCV2	feedback	hand-writing	2	546055	136371	var	var	var	3
21	Homer	AutoCV2	feedback	action	12	1354	353	var	var	var	3
22	Isaac2	AutoCV2	feedback	action	249	38372	9561	var	102	78	1
23	Formula	AutoCV2	feedback	miscellaneous	4	32994	8203	var	80	80	3
24	Apollon	AutoCV2	final	people	100	6077	1514	1	var	var	3
25	Loukoum	AutoCV2	final	hand-writing	3	27938	6939	1	var	var	3
26	Fiona	AutoCV2	final	action	6	8038	1962	var	var	var	3
27	Monica1	AutoCV2	final	action	20	10380	2565	var	168	168	3
28	Kitsune	AutoCV2	final	action	25	18602	4963	var	46	82	3

dataset formatting toolkit available at: https://github.com/zhengying-liu/autodl-contrib

Liu Z, Xu Z, Escalera S, Guyon I, Treguer S, Tu W-W. Towards Automated Computer Vision: Analysis of the AutoCV Challenges 2019. :7.

Evaluation

- Multiple predictions to make
- ROC AUC
- Area under Learning Curve (ALC)
- Average rank



Evaluation



Participation

challenge name	Collocated with	#participants	#submission s	begin date (2019)	end date (2019)
AutoCV	IJCNN	102	938	May 1	Jun 29
AutoCV2	ECML PKDD	34	336	July 2	Aug 20
AutoNLP	WAIC	66	420	Aug 2	Aug 31
AutoSpeech	ACML	33	234	Sep 16	Oct 16
AutoWSL	ACML	26	439	Sep 24	Oct 29

Winners

Challenge	1st place	2rd place	3nd place
	(\$2000)	(\$1500)	(\$500)
AutoCV	kakaobrain	DKKimHCLee	base_1
	(Kakao Brain)	(Hana. Tech. Inst.)	(Hanyang University)
AutoCV2	kakaobrain	tanglang	kvr
	(Kakao Brain)	(Xiamen University)	(-)
AutoNLP	DeepBlueAl	upwind_flys	txta
	(DeepBlue Technology)	(Lenovo)	(gsdata.cn)
AutoSpeech	PASA_NJU	DeepWisdom	Kon
	(Nanjing University)	(fuzhi.ai)	(NS Solutions Corporation)
AutoWSL	DeepWisdom	Meta_Learners	lhg1992
	(fuzhi.ai)	(Tsinghua University)	(inspur.com)

All winners' code is now open-sourced on GitHub

URLs can be found on: autodl.chalearn.org

Leaderboard overfitting

Average rank - feedback vs final



No leaderboard overfitting => universal AutoML solutions

Dataset difficulty



Any-time learning problem



Some teams have good final performance but bad any-time performace => any-time learning aspect to be studied further

Conclusion

Exploration-exploitation trade-off: keep it in mind!

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

AutoDL challenge still on-going!

Theoretical possibility of AutoML

Can we beat "No Free Lunch"? Why? How?

Computational considerations

Statistical vs Computational trade-off: what's the limit?

Theoretical guarantee of ensemble methods

Rigorous mathematical proof of the effectiveness of ensemble methods



Automated Deep Learning

LIU Zhengying U. Paris-Sud / Inria / U. Paris Saclay

Thank you! Questions?

Internship opportunities:

1. AutoDL Benchmark with extensive GPU usage

2. Meta-learning challenge design and implementation Contact: <u>zhengying.liu@inria.fr</u>