Automated Machine Learning – An Introduction to Network Architecture Search

Lecture 8 for Advanced Deep Learning Systems

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Introduction

Introduction

During the last lecture, we explored optimizing our network through informed manual adjustments. Today, we'll delve into Automated Machine Learning and the process of Network Architecture Search.

Introduction - Automated Machine Learning

The complete AutoML pipeline consists of:

- Data preparation and automated data cleaning
- Feature Engineering
- Model selection or Network Architecture Search
- Hyperparameter tuning ...

Introduction - Network Architecture Search

Core idea: Can we design the best network architecture purely from observing the data?

We want to pick the optimal architecture $a \in \mathcal{A}$ from a set of architectures $\mathcal{A}$.

At the same time, we want to pick the optimal parameters $w^*(a)$ for the architecture a.

$$\begin{aligned} min_{a \in \mathcal{A}} \mathcal{L}_{val}(w^*(a), a) \\ s.t. w^*(a) = argmin_w(\mathcal{L}_{train}(w, a)) \end{aligned} \tag{1}$$

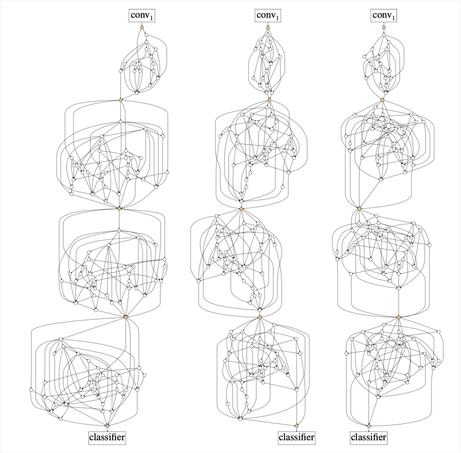
Search Space

What is a search space?

We normally have to search through a given set of architectures $\mathcal{A}$, which is known as the search space.

- Global search space
- Modular search space
- Combined search space

Global search space



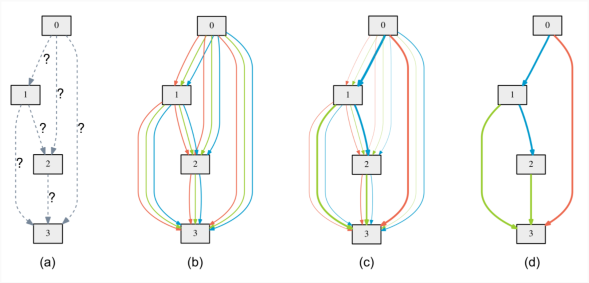
A global search space considers directly all possible elements (search options) in the DAG (Directed Acyclic Graph): this is an extremely large search space, not even tractable.

Modular search space

- Search a critical component in the search space, and then duplicate that component based on heuristics (DARTS).
- Template and backbone template with heuristics, search for the design options in the backbone (MobileNet-V3).

The DARTS search space

- 6-node DAG as a Cell
  - two input nodes
  - one output node
  - four intermediate data nodes
- Nodes are connected by an operation
  - conv3x3
  - conv1x1
  - skip, relu, sigmoid, tanh and so on.
- roughly 10^9 options



The DARTS search space

- Normal Cell (no resolution change)
- Reduction Cell (resolution changes with striding/pooling)

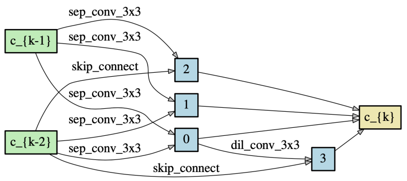


Figure 4: Normal cell learned on CIFAR-10.

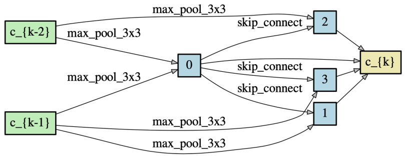
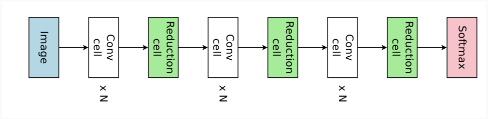


Figure 5: Reduction cell learned on CIFAR-10.

The DARTS search space

- Searched on CIFAR10 with one normal and one reduction cell.
- There exists an approximation/belief that architectures learned on CIFAR10 are generally transferrable to other image tasks!
- Stack the searched cell multiple times to build bigger networks on ImageNet.
- There exists a heuristics-defined stacking pattern! Figure is from ENAS but DARTS does the same thing.

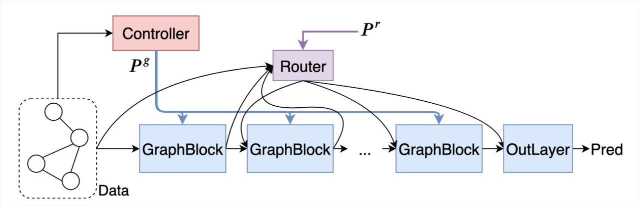


Combined search space

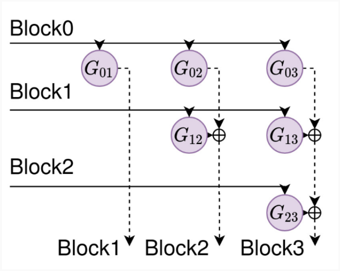
- Micro-architecture design: the design of a single cell, through the modular search space.
- Macro-architecture design: how these cells should be connected, through the global search space.
- The decomposition makes the total search space smaller and more tractable.

Combined search space

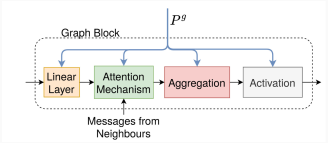
Combined search space



Macro-architecture



Micro-architecture



Search Strategies

What is a search strategy?

The core-algorithm used to conduct the search.

- Reinforcement learning
- Gradient-based optimization
- Evolutionary Algorithm
- Performance estimator

Reinforcement Learning based NAS (NASNet)

A controller, parameterized by θ_c performs a list of actions $(a_0, a_1 ... a_{T-1})$ to design the architecture of a child network.

The child network achieves an accuracy R on a held-out validation dataset.

Concretely, the controller is optimizing a reward:

$$J(\theta_c) = E_{P(\{a_0,\ldots,a_{T-1}\},\theta_c)}[R] \tag{2}$$

Reinforcement Learning based NAS (NASNet)

The reward signal R is non-differentiable, so we use a policy gradient to iteratively update θ_c

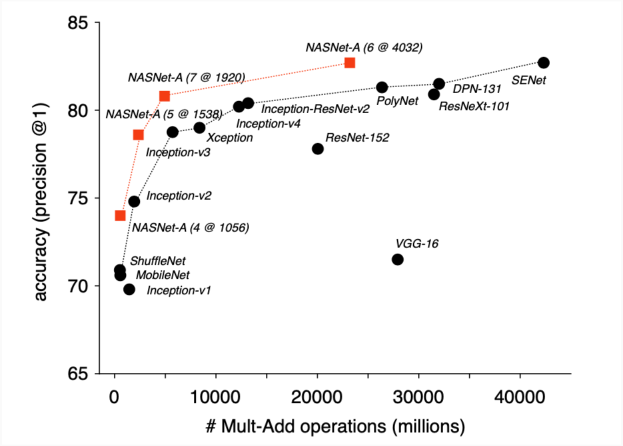
$$J(\theta_c) = \frac{1}{M} \sum_{k=0}^{M-1} \sum_{t=0}^{T-1} logP(a_t | \{a_{t-1} ... a_0\}; \theta_c) R \tag{3}$$

Where M is the number of different architectures that the controller samples in one batch and T is the number of hyperparameters our controller has to predict to design a neural network architecture.

This is slightly different from standard RL setup since there is only basically two states (start and finish) in the trajectory.

It requires a full-training run to obtain R, so this is very expensive!

Reinforcement Learning based NAS (NASNet)



Gradient-based NAS (DARTs)

The problem with RL-based NAS is that it is hard for the controller to receive gradients that relates to the child network accuracy.

But what if we can make the operators differentiable?

Gradient-based NAS (DARTs)

We associate each operator with a trainable parameter:

Let O be a set of candidate operators (eg. convolution, max pool ...), To make a continuous search space, one can relax the discrete categorical distribution:

$$\bar{o}^{(i,j)}(x) = \sum_{o \in O} \frac{exp(\alpha_o^{(i,j)})}{\sum_{o' \in O} exp(\alpha_{o'}^{(i,j)})} o(x) \tag{4}$$

The operation mixing weights for a pair of nodes (i, j) are parameterized by a vector $\alpha(i, j)$ of dimension $|O|$.

Translate this to words: weighting each operator using trainable α values.

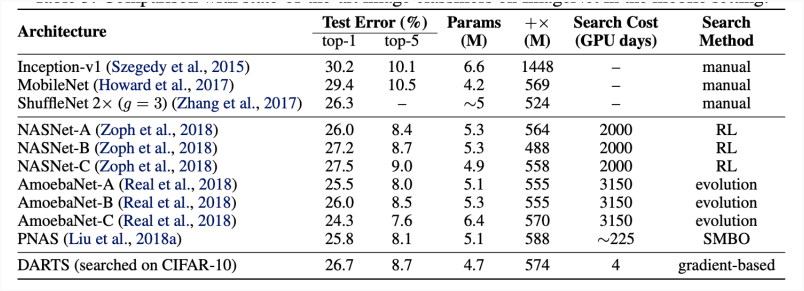
Gradient-based NAS (DARTs)

- Update architecture α by descending $\nabla_\alpha L_{\text{val}}(w - \xi \nabla_w L_{\text{train}}(w, \alpha), \alpha)$, ξ is zero for first order optimization)
- Update weights w by descending $\nabla_w L_{\text{train}}(w, \alpha)$
- Derive the final architecture based on the learned α.

Dual-level optimization using SGD.

Gradient-based NAS (DARTs)

Significant time reduction, since now we run search on the cell-based space only once! There is now no need for evaluating each child network



Architecture	Test Error (%)		Params (M)	$+\times$ (M)	Search Cost (GPU days)	Search Method
	top-1	top-5				
Inception-v1 (Szegedy et al., 2015)	30.2	10.1	6.6	1448	–	manual
MobileNet (Howard et al., 2017)	29.4	10.5	4.2	569	–	manual
ShuffleNet 2× ($g = 3$) (Zhang et al., 2017)	26.3	–	∼5	524	–	manual
NASNet-A (Zoph et al., 2018)	26.0	8.4	5.3	564	2000	RL
NASNet-B (Zoph et al., 2018)	27.2	8.7	5.3	488	2000	RL
NASNet-C (Zoph et al., 2018)	27.5	9.0	4.9	558	2000	RL
AmoebaNet-A (Real et al., 2018)	25.5	8.0	5.1	555	3150	evolution
AmoebaNet-B (Real et al., 2018)	26.0	8.5	5.3	555	3150	evolution
AmoebaNet-C (Real et al., 2018)	24.3	7.6	6.4	570	3150	evolution
PNAS (Liu et al., 2018a)	25.8	8.1	5.1	588	∼225	SMBO
DARTS (searched on CIFAR-10)	26.7	8.7	4.7	574	4	gradient-based

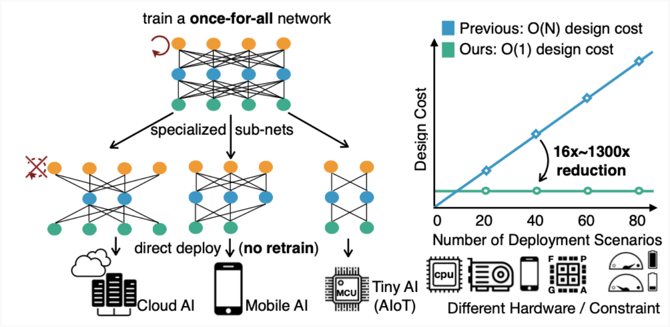
Evolutionary Algorithm (OFA)

Gradient-based methods suffer from the following problems

- Large VRAM usage (Single-path method)
- Is the ranking on a proxy dataset reliable?
- Gradient interference (PC-DARTs)
- No awareness about the deployment device and scenarios

Evolutionary Algorithm (OFA)

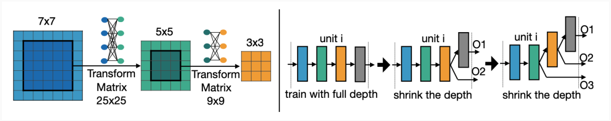
What if we train a supernet, and subsample it?

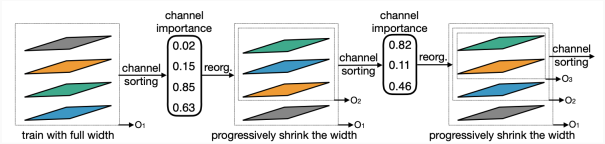

train a **once-for-all** network
specialized sub-nets
direct deploy (**no retrain**)
Cloud AI
Mobile AI
MCU
Tiny AI (AIoT)
Previous: O(N) design cost
Ours: O(1) design cost
Design Cost
16x~1300x reduction
0
20
40
60
80
Number of Deployment Scenarios
cpu
Different Hardware / Constraint

Evolutionary Algorithm (OFA)

Design a large supernet that supports sub-sampling in various dimensions

- Kernels
- Channels
- Layers





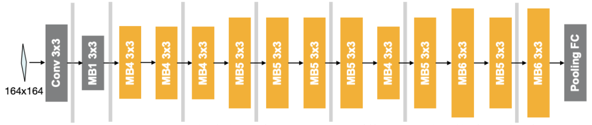
Evolutionary Algorithm (OFA)

Then use an evolutionary algorithm to traverse the whole search space.

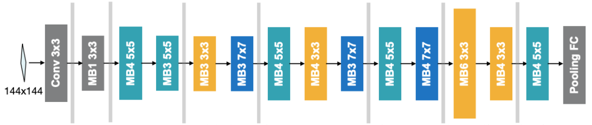
- **Initialization and Evaluation:** At the start, generate a random population of individuals, and evaluate their performance
- **Selection:** Individuals are selected based on their fitness scores.
- **Crossover:** Selected individuals pair and exchange parts of their structure, creating a new individual called offspring. This process is also known as recombination or mating.
- **Mutation:** Offspring are altered randomly to introduce variability in the population. This prevents the genetic algorithm from stagnating at local optima.
- **Replacement:** The population is updated with the new offspring, usually replacing the least fit individuals. The algorithm then goes back to the evaluation step, creating a loop.

Evolutionary Algorithm (OFA)

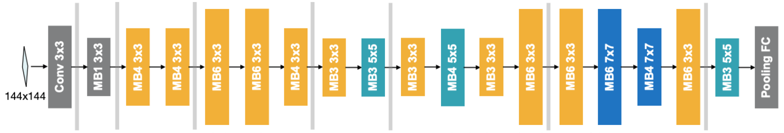
Do the search with different hardware targets, use the latency and accuracy to build a fitness score



(a) 4.1ms latency on Xilinx ZU3EG (batch size = 1).



(b) 10.9ms latency on Intel Xeon CPU (batch size = 1).

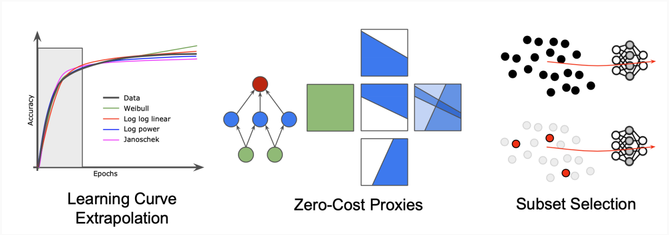


(c) 14.9ms latency on NVIDIA 1080Ti (batch size = 64).

Performance Predictor (Speedy Performance Estimator)

All previous methods require training of one or more networks. Can we predict the performance without or with minimal training?

- Learning curve extrapolation: extrapolating the validation accuracy learning curve via a parameteric model.
- Zero-cost proxies: assessing the generalizability of an architecture with a single forward pass of a single minibatch of data
- Subset selection: Training the architecture on a subset of the data



Performance Predictor (Speedy Performance Estimator)

An example performance predictor can be the following: Let L denote a loss function, $f_\theta(x)$ the output of a neural network f with input x and parameters θ, and let $\theta_{t,i}$ denote the parameters of the network after t epochs and i minibatches of SGD.

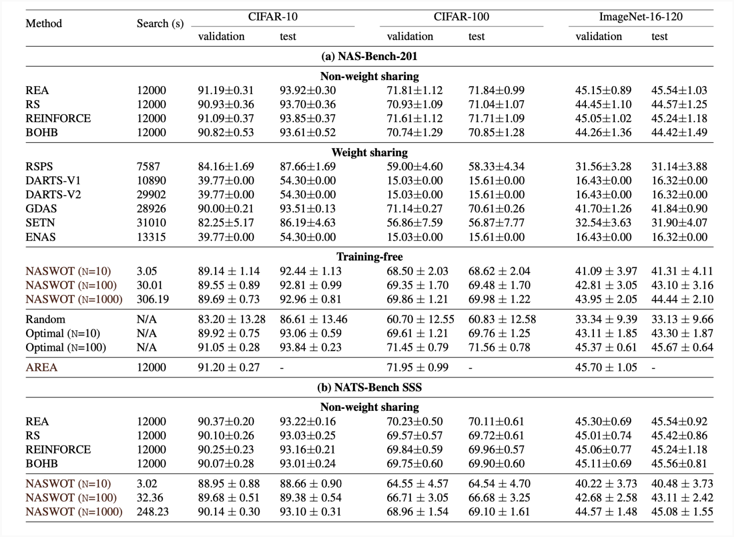
After training the network for T epochs, we sum the training losses collected so far to get the following Training Speed Estimate (TSE)

$$TSE = \sum_{t=1}^{T} [\frac{1}{B} \sum_{1}^{B} L(f_{\theta_{t,i}(x_i),y_i})] \tag{5}$$

The idea is then use this for evaluating the sub-networks, since it gets a better rank correlation performance usually.

Performance Predictor (NASWOT)

Or you can simply take a number of networks and evaluate all of them using these low-fidelity proxies!



Method	Search (s)	CIFAR-10		CIFAR-100		ImageNet-16-120	
		validation	test	validation	test	validation	test
(a) NAS-Bench-201							
Non-weight sharing							
REA	12000	91.19±0.31	93.92±0.30	71.81±1.12	71.84±0.99	45.15±0.89	45.54±1.03
RS	12000	90.93±0.36	93.70±0.36	70.93±1.09	71.04±1.07	44.45±1.10	44.57±1.25
REINFORCE	12000	91.09±0.37	93.85±0.37	71.61±1.12	71.71±1.09	45.05±1.02	45.24±1.18
BOHB	12000	90.82±0.53	93.61±0.52	70.74±1.29	70.85±1.28	44.26±1.36	44.42±1.49
Weight sharing							
RSPS	7587	84.16±1.69	87.66±1.69	59.00±4.60	58.33±4.34	31.56±3.28	31.14±3.88
DARTS-V1	10890	39.77±0.00	54.30±0.00	15.03±0.00	15.61±0.00	16.43±0.00	16.32±0.00
DARTS-V2	29902	39.77±0.00	54.30±0.00	15.03±0.00	15.61±0.00	16.43±0.00	16.32±0.00
GDAS	28926	90.00±0.21	93.51±0.13	71.14±0.27	70.61±0.26	41.70±1.26	41.84±0.90
SETN	31010	82.25±5.17	86.19±4.63	56.86±7.59	56.87±7.77	32.54±3.63	31.90±4.07
ENAS	13315	39.77±0.00	54.30±0.00	15.03±0.00	15.61±0.00	16.43±0.00	16.32±0.00
Training-free							
NASWOT (N=10)	3.05	89.14 ± 1.14	92.44 ± 1.13	68.50 ± 2.03	68.62 ± 2.04	41.09 ± 3.97	41.31 ± 4.11
NASWOT (N=100)	30.01	89.55 ± 0.89	92.81 ± 0.99	69.35 ± 1.70	69.48 ± 1.70	42.81 ± 3.05	43.10 ± 3.16
NASWOT (N=1000)	306.19	89.69 ± 0.73	92.96 ± 0.81	69.86 ± 1.21	69.98 ± 1.22	43.95 ± 2.05	44.44 ± 2.10
Random	N/A	83.20 ± 13.28	86.61 ± 13.46	60.70 ± 12.55	60.83 ± 12.58	33.34 ± 9.39	33.13 ± 9.66
Optimal (N=10)	N/A	89.92 ± 0.75	93.06 ± 0.59	69.61 ± 1.21	69.76 ± 1.25	43.11 ± 1.85	43.30 ± 1.87
Optimal (N=100)	N/A	91.05 ± 0.28	93.84 ± 0.23	71.45 ± 0.79	71.56 ± 0.78	45.37 ± 0.61	45.67 ± 0.64
AREA	12000	91.20 ± 0.27	-	71.95 ± 0.99	-	45.70 ± 1.05	-
(b) NATS-Bench SSS							
Non-weight sharing							
REA	12000	90.37±0.20	93.22±0.16	70.23±0.50	70.11±0.61	45.30±0.69	45.54±0.92
RS	12000	90.10±0.26	93.03±0.25	69.57±0.57	69.72±0.61	45.01±0.74	45.42±0.86
REINFORCE	12000	90.25±0.23	93.16±0.21	69.84±0.59	69.96±0.57	45.06±0.77	45.24±1.18
BOHB	12000	90.07±0.28	93.01±0.24	69.75±0.60	69.90±0.60	45.11±0.69	45.56±0.81
NASWOT (N=10)	3.02	88.95 ± 0.88	88.66 ± 0.90	64.55 ± 4.57	64.54 ± 4.70	40.22 ± 3.73	40.48 ± 3.73
NASWOT (N=100)	32.36	89.68 ± 0.51	89.38 ± 0.54	66.71 ± 3.05	66.68 ± 3.25	42.68 ± 2.58	43.11 ± 2.42
NASWOT (N=1000)	248.23	90.14 ± 0.30	93.10 ± 0.31	68.96 ± 1.54	69.10 ± 1.61	44.57 ± 1.48	45.08 ± 1.55

Is This A Solved Problem?

Well, Yes and No

- Search spaces are normally manually defined!
- Low-fidelity methods normally work at small search spaces.
- Many of the search methods actually overfit to the search space!

Summary

Search Spaces: Global, Modular and Combined

Search Strategies

- Reinforcement learning
- Gradient-based optimization
- Evolutionary algorithm
- Performance estimators