Neural Architecture Search

REDS

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Overview

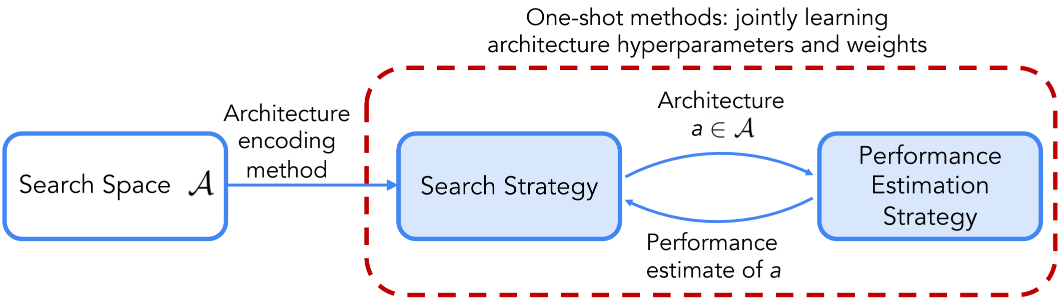


Figure: Overview of NAS.

A search strategy iteratively selects architectures (typically by using an architecture encoding method) from a predened search space $\mathcal{A}$.

The architectures are passed to a performance estimation strategy, which returns the performance estimate to the search strategy.

For one-shot methods, the search strategy and performance estimation strategy are inherently coupled.

Search space

Definition

The set of all architectures that the NAS algorithm is allowed to select.

- Size: from a few thousand to over 10^{20}.
- Reduction: adding domain knowledge.

$\rightarrow$ Introduce humain bias $\rightarrow$ x reduce the chance of finding truly nover architecture.

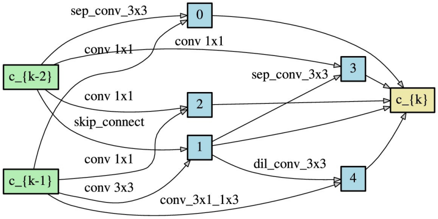


Figure: Architecture directed acyclic graph (DAG) with operation on nodes

Search strategy

Definition

The optimization technique used to find a high-performing architecture in the search space.

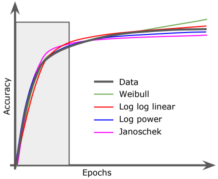
- Black-box optimization techniques : RL, Bayesian optimization, evolutionary search.
- One-shot techniques: supernet-hypernet based methods.

Performance estimation strategy

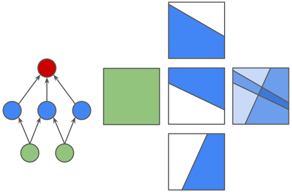
Definition

Any method used to quickly predict the performance of neural architectures in order to avoid fully training the architecture.

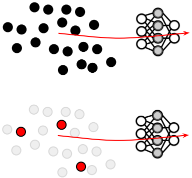
- Full training & evaluation.
- Performance estimation strategy.



Learning Curve Extrapolation



Zero-Cost Proxies



Subset Selection

Benchmarks

Definition

A NAS benchmark is defined as a dataset with a fixed train-test split, a search space, and a fixed evaluation pipeline for training the architectures.

- Tabular benchmarks: precomputed evaluations for all possible architecture in the search space.

$\rightarrow$ Allow to **simulate** hundreds of trials !
  - No more training.
  - Statistically significant comparisons (simulation with multiple seeds).
- Specialization: precomputed evaluation for NLP tasks, protein folding, astronomy imaging, for vision dataset (CIFAR-10(0), ImageNet, ...)
- Most popular NAS benchmarks
  - NAS-Bench-101/202
  - Surr-NAS-Bench-DARTS
  - TransNAS-Bench-101
  - NAS-Bench-Suite

Evalutation

Table 2: **Comparison with Transferable NAS on NB201 Serach Space.** We present the accuracy achieved on four unseen datasets. Additionally, we provide the number of neural architectures (**Trained Archs**) that are actually trained to achieve accuracy. The accuracies are reported with 95% confidence intervals over 3 runs.

Type	Method	CIFAR-10 Accuracy (%)	CIFAR-10 Trained Archs	CIFAR-100 Accuracy (%)	CIFAR-100 Trained Archs	Aircraft Accuracy (%)	Aircraft Trained Archs	Oxford-IIIT Pets Accuracy (%)	Oxford-IIIT Pets Trained Archs
	ResNet (He et al., 2016)	$93.97_{\pm 0.00}$	N/A	$70.86_{\pm 0.00}$	N/A	$47.01_{\pm 1.16}$	N/A	$25.58_{\pm 3.43}$	N/A
	RS (Bergstra & Bengio, 2012)	$93.70_{\pm 0.36}$	> 500	$71.04_{\pm 1.07}$	> 500	-	-	-	-
	REA (Real et al., 2019)	$93.92_{\pm 0.30}$	> 500	$71.84_{\pm 0.99}$	> 500	-	-	-	-
	REINFORCE (Williams, 1992)	$93.85_{\pm 0.37}$	> 500	$71.71_{\pm 1.09}$	> 500	-	-	-	-
One-shot NAS*	RSPS (Li & Talwalkar, 2019)	$84.07_{\pm 3.61}$	N/A	$52.31_{\pm 5.77}$	N/A	$42.19_{\pm 3.88}$	N/A	$22.91_{\pm 1.65}$	N/A
	SETN (Dong & Yang, 2019a)	$87.64_{\pm 0.00}$	N/A	$59.09_{\pm 0.24}$	N/A	$44.84_{\pm 3.96}$	N/A	$25.17_{\pm 1.68}$	N/A
	GDAS (Dong & Yang, 2019b)	$93.61_{\pm 0.09}$	N/A	$70.70_{\pm 0.30}$	N/A	$53.52_{\pm 0.48}$	N/A	$24.02_{\pm 2.75}$	N/A
	PC-DARTS (Xu et al., 2020)	$93.66_{\pm 0.17}$	N/A	$66.64_{\pm 2.34}$	N/A	$26.33_{\pm 3.40}$	N/A	$25.31_{\pm 1.38}$	N/A
	DrNAS (Chen et al., 2021)	$94.36_{\pm 0.00}$	N/A	$\mathbf{73.51_{\pm 0.00}}$	N/A	$46.08_{\pm 7.00}$	N/A	$26.73_{\pm 2.61}$	N/A
BO-based NAS	BOHB (Falkner et al., 2018)	$93.61_{\pm 0.52}$	> 500	$70.85_{\pm 1.28}$	> 500	-	-	-	-
	GP-UCB	$\mathbf{94.37_{\pm 0.00}}$	58	$73.14_{\pm 0.00}$	100	$41.72_{\pm 0.00}$	40	$40.60_{\pm 1.10}$	11
	BANANAS (White et al., 2021a)	$\mathbf{94.37_{\pm 0.00}}$	46	$\mathbf{73.51_{\pm 0.00}}$	88	$41.72_{\pm 0.00}$	40	$40.15_{\pm 1.59}$	17
	NASBOWL (Ru et al., 2021)	$94.34_{\pm 0.00}$	100	$\mathbf{73.51_{\pm 0.00}}$	87	$53.73_{\pm 0.83}$	40	$41.29_{\pm 1.10}$	17
	HEBO (Cowen-Rivers et al., 2022)	$94.34_{\pm 0.00}$	100	$72.62_{\pm 0.20}$	100	$49.32_{\pm 6.10}$	40	$40.55_{\pm 1.15}$	18
Transferable NAS	TNAS (Shala et al., 2023)	$\mathbf{94.37_{\pm 0.00}}$	29	$\mathbf{73.51_{\pm 0.00}}$	59	$59.15_{\pm 0.58}$	26	$40.00_{\pm 0.00}$	6
	MetaD2A (Lee et al., 2021a)	$\mathbf{94.37_{\pm 0.00}}$	100	$73.34_{\pm 0.04}$	100	$57.71_{\pm 0.20}$	40	$39.04_{\pm 0.20}$	40
	DiffusionNAG (Ours)	$\mathbf{94.37_{\pm 0.00}}$	**5**	$\mathbf{73.51_{\pm 0.00}}$	**5**	$\mathbf{59.63_{\pm 0.92}}$	**2**	$\mathbf{41.32_{\pm 0.84}}$	**2**

Figure: Result table example

Evalutation

Table 8
Comparison of the evaluation results on CIFAR-10 and CIFAR-100.

Architecture	Test Err. (%)		Params	Search Cost	Search
	C-10	C-100	(.M)	(GPU-days)	Method
NASNet-A [8]	2.65	-	3.3	1800	RL
AmoebaNet-A [20]	3.34	-	3.2	3150	Evolution
PNAS [40]	3.41	-	3.2	225	SMBO
RelativeNAS [41]	2.34	15.86	3.93	0.4	Evolution
DARTS (first order) [10]	3	17.76	3.3	1.5	Gradient
SNAS + mild constraint [42]	2.98	-	2.9	1.5	Gradient
ProxylessNAS [29]	2.08	-	5.7	4	Gradient
P-DARTS† (C-10) [18]	2.5	16.55	3.4	0.3	Gradient
P-DARTS† (C-100) [18]	2.62	15.92	3.6	0.3	Gradient
P-DARTS† (C-10-Large) [18]	2.25	15.27	10.5	0.3	Gradient
P-DARTS† (C-100-Large) [18]	2.43	14.64	11	0.3	Gradient
Ours† (`C-10`)	2.47 ± 0.03	-	2.04	$1.3^{\star}$	RL
Ours† (`C-100`)	2.58 ± 0.05	-	3.43	$1.3^{\star}$	RL
Ours† (`C-10-Large`)	-	15.3 ± 0.04	9.57	$1.3^{\star}$	RL
Ours† (`C-100-Large`)	-	14.6 ± 0.03	10.5	$1.3^{\star}$	RL

Figure: Result table example

Contribution

- Problem: Classical NAS need to train thousand of architecture.

$\rightarrow$ Switch from searching architecture to directly generate architecture using a graph diffusion model.

$\rightarrow$ diffusionNAG

Contribution

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Limits

- Need to retrain f_Φ for every metrics
  - Accuracy
  - Inference time
  - Memory usage
  - Adversarial attack resistance
  - ...
- Only one metric is optimized: no compromise possible
- Linear combination of metrics: not ideal to find a good compromise

Our contrib title

Heading

- Train a multi-objective predictor using the same task aware dataset, but enhanced with metrics of interest
- Guide the diffusion with the multi-objective predictor:
  - Generate a bigger super-network with disableable blocks
  - ie: equal to an encoding of points near the pareto front (best possible compromise between metrics)
- Constraints encoding within the same score network
  - Layer compatibility in a block
  - Compatibility between blocks inputs and outputs

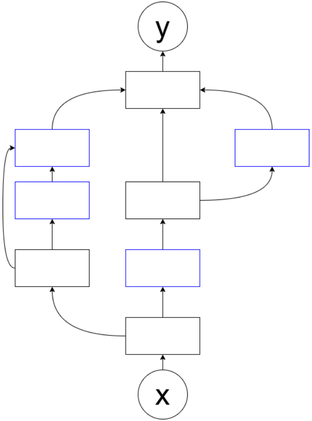

Figure: Example of disableable architecture

- Train the obtained super-network after diffusion inference
- Disable the blocks depending on the metrics of interest

Advantages and limits of this approach

- Flexibility for the user : fix the metrics threshold only after performing the NAS
- Dynamic architecture depending on external parameters
- But :
  - Predictor needs to be retrained if a new metric is added
  - Diffusion inference more costly
  - No guarantees if the pareto optimality is well covered by the disableable blocks

Evaluation and results

Two evaluations

- Achitecture search
- generated architecture performances
- generation cheaper than previous full space search
- multi-objective benchmarks for the obtained architectures

Results for a classifier model on CIFAr-10			
Model	Ours	DiffusionNAG	(egrg) best RL methods
architecture search time (min)	23.6	544	¿ 2000
Inference costs of the generated architecture (MFLOPs)	250	434	670

References

John Smith (2012)
Title of the publication
Journal Name 12(3), 45 – 678.

Thank you