Neural Architecture Search

REDS

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Overview

Overview of NAS

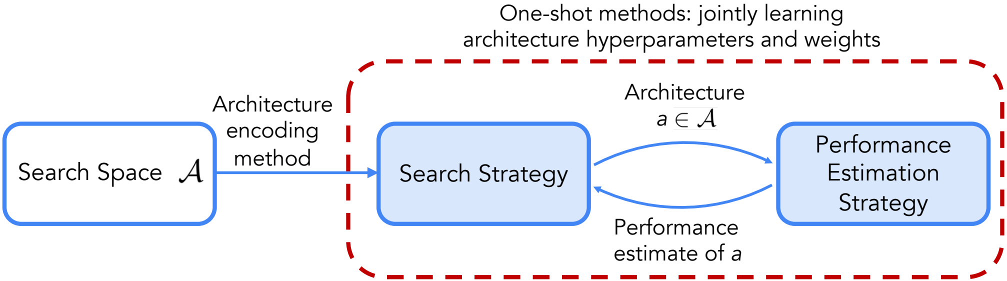


Figure: Overview of NAS.
A search strategy iteratively selects architectures (typically by using an architecture encoding method) from a predened search space $\mathcal{A}$.
The architectures are passed to a performance estimation strategy, which returns the performance estimate to the search strategy.
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.

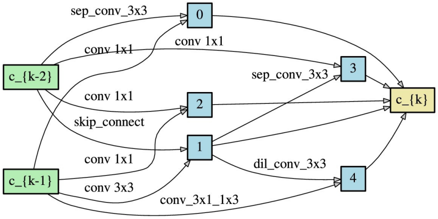


Figure: Architecture directed acyclic graph (DAG) with operation on nodes

Type of Search Space

Search Spaces	Structure	Searchable hyperparameters
Macro search space	DAG	Operation types, DAG topology macro hyperparameters
Chain-structured search space	Chain	Operation types, macro hyperparameters
Cell-based search space	Duplicated cells	Operation type, cell topology
Hierarchical search space	Varied	Operation type, cell/DAG topology macro hyperparameters

Table: Type of Search Space

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.

Taxonomy and One shot methods

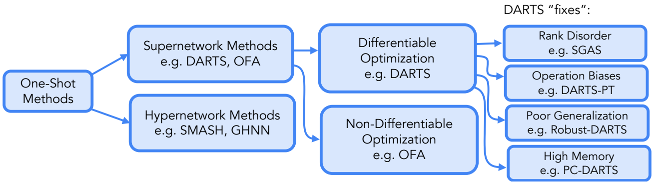


Figure: Taxonomy of one shot methods.

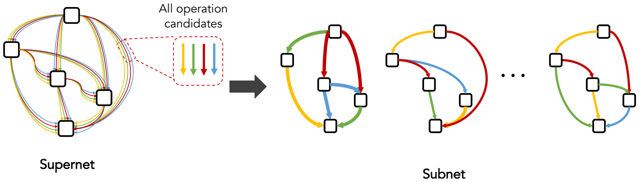


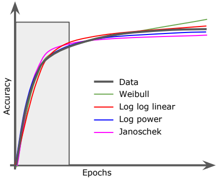
Figure: Supernetwork

Performance estimation strategy

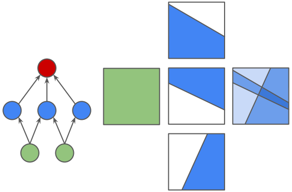
Definition

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

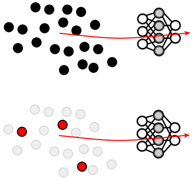
- Full training & evaluation.
- Performance estimation strategy.



Learning Curve Extrapolation



Zero-Cost Proxies



Subset Selection

Evaluation: 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$0.00	N/A	**73.51$\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$1.28	> 500	-	-	-	-
	GP-UCB	**94.37$\pm$0.00**	58	73.14$\pm$0.00	100	41.72$\pm$0.00	40	40.60$\pm$1.10	11
	BANANAS (White et al., 2021a)	**94.37$\pm$0.00**	46	**73.51$\pm$0.00**	88	41.72$\pm$0.00	40	40.15$\pm$1.59	17
	NASBOWL (Ru et al., 2021)	94.34$\pm$0.00	100	**73.51$\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$1.15	18
Transferable NAS	TNAS (Shala et al., 2023)	**94.37$\pm$0.00**	29	**73.51$\pm$0.00**	59	59.15$\pm$0.58	26	40.00$\pm$0.00	6
	MetaD2A (Lee et al., 2021a)	**94.37$\pm$0.00**	100	73.34$\pm$0.04	100	57.71$\pm$0.20	40	39.04$\pm$0.20	40
	DiffusionNAG (Ours)	**94.37$\pm$0.00**	**5**	**73.51$\pm$0.00**	**5**	**59.63$\pm$0.92**	**2**	**41.32$\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. (%) C-10	Test Err. (%) C-100	Params (.M)	Search Cost (GPU-days)	Search 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

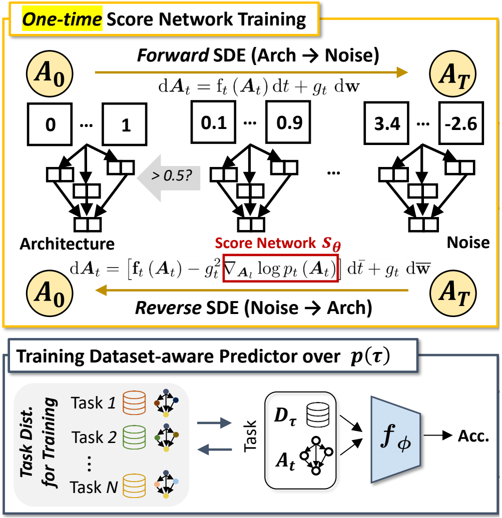
Contribution: base

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

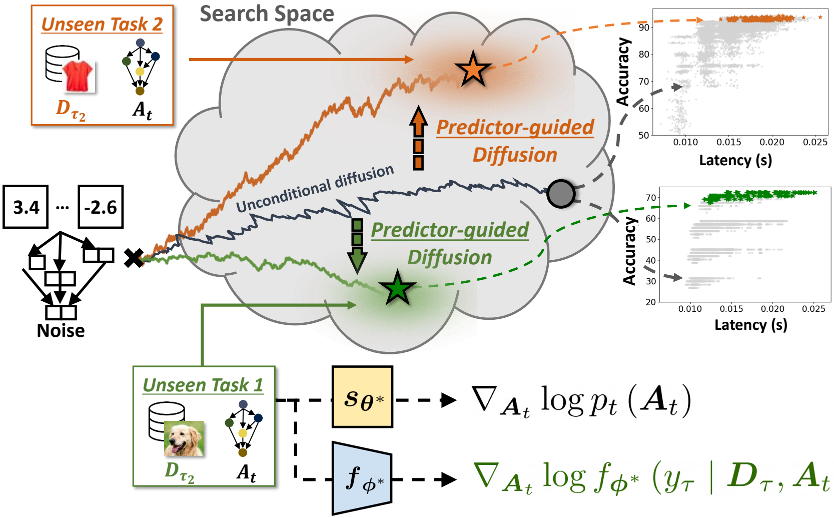
→ Switch from searching architecture to directly generate architecture using a graph diffusion model.

→ diffusionNAG

Contribution: diffusionNAG



Contribution: diffusionNAG



$$\nabla_{A_t} \log p_t(A_t)$$

$$\nabla_{A_t} \log f_{\phi^*}(y_\tau \mid D_\tau, A_t)$$

Contribution: diffusionNAG

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

Contribution: MOD-NAG

Multi-Objective Diffusion Neural Architecture Search

- 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

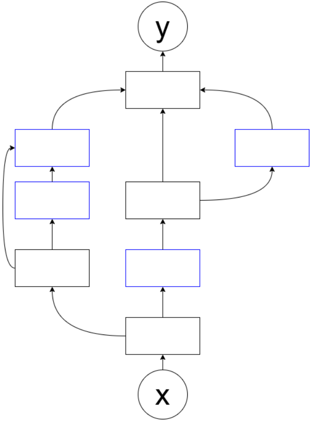
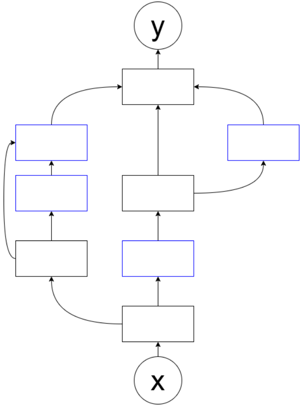
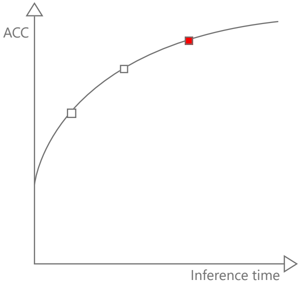


Figure: Example of disableable architecture

Contribution: MOD-NAG

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





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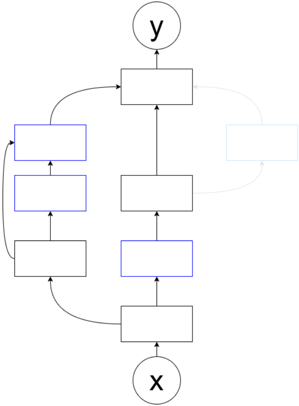

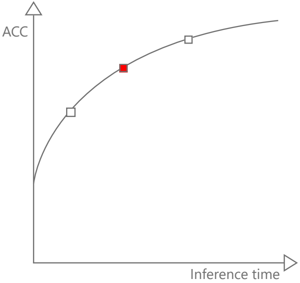

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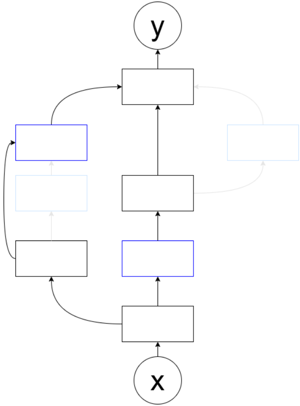

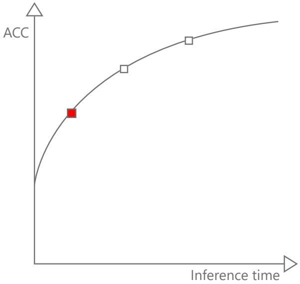

Advantages and limits of this approach

- 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

- Architecture search
- Generated architecture performances

Comparison with other methods

- Generation cheaper than previous full space search
- Multi-objective benchmarks for the obtained architectures

Results

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

Architecture	Test Err. (%)	Params (.M)	Search Cost (GPU-days)	Search Method
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DiffusionNAG (C-100)	2.58 ± 0.05	3.43	1.3*	Diffusion
MOD-NAG (C-10)	2.78 ± 0.04	2.04	1.8*	Diffusion
MOD-NAG (C-100)	3.11 ± 0.07	3.43	1.8*	Diffusion

References

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Thank you