香港中文大學
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CMSC5743

L09: Network Architecture Search

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Overview

Search Space Design

Blackbox Optimization

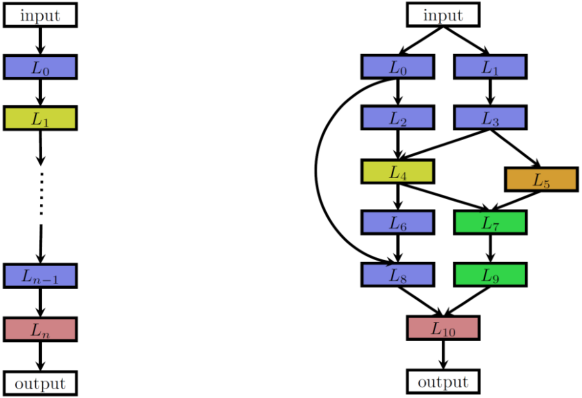
- NAS as a hyperparameter optimization
- Reinforcement Learning
- Evolution methods
- Regularized methods
- Baysian Optimization
- Differentiable search
- Efficient methods

NAS Benchmark

Estimation strategy

Overview

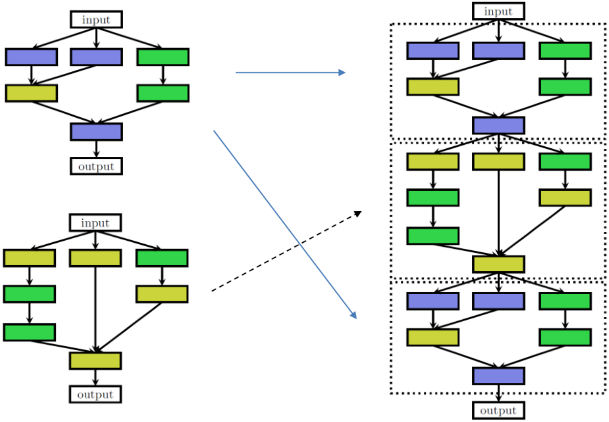
Basic architecture search



Each node in the graphs corresponds to a layer in a neural network [1]

[1] Thomas Elsken, Jan Hendrik Metzen, and Frank Hutter (2018). "Neural architecture search: A survey". In: *arXiv preprint arXiv:1808.05377*

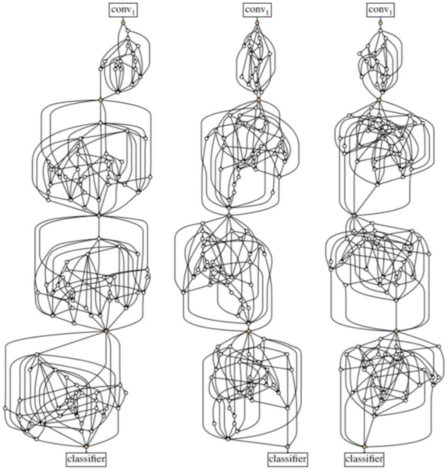
Cell-based search



Normal cell and reduction cell can be connected in different order[2]

[2] Thomas Elsken, Jan Hendrik Metzen, and Frank Hutter (2018). “Neural architecture search: A survey”. In: *arXiv preprint arXiv:1808.05377*

Graph-based search space



Randomly wired neural networks generated by the classical Watts-Strogatz model [3]

[3] Saining Xie et al. (2019). "Exploring randomly wired neural networks for image recognition". In: *Proceedings of the IEEE International Conference on Computer Vision*, pp. 1284–1293

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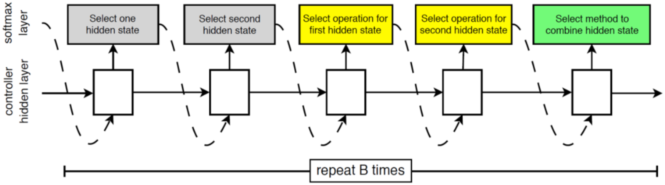
NAS as hyperparameter optimization



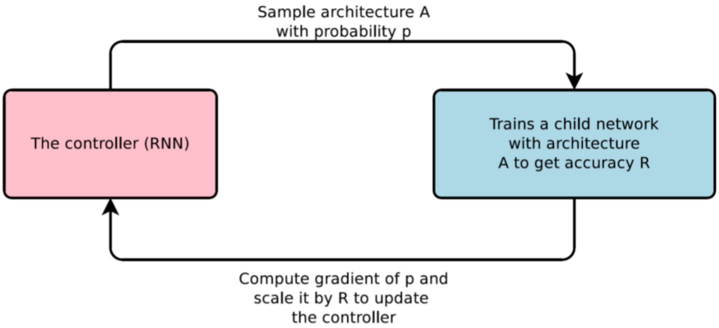
Controller architecture for recursively constructing one block of a convolutional cell [4]

Features

- 5 categorical choices for N^{th} block
  - 2 categorical choices of hidden states, each with domain $0, 1, ..., N-1$
  - 2 categorical choices of operations
  - 1 categorical choices of combination method
  - Total number of hyperparameters for the cell: 5B (with B = 5 by default)
- Unstricted search space
  - Possible with conditional hyperparameters
    (but only up to a prespectified maximum number of layers)
  - Example: chain-structured search space
    - Top-level hyperparameter: number of layers L
    - Hyperparameters of layer K conditional on $L \geq k$

[4] Barret Zoph, Vijay Vasudevan, et al. (2018). "Learning transferable architectures for scalable image recognition". In: *Proceedings of the IEEE conference on*

Reinforcement learning



Overview of the reinforcement learning method with RNN [5]

Reinforcement learning with a RNN controller

- State-of-the-art results for CIFAR-10, Penn Treebank
- Large computation demands
  800 GPUs for 3-4 weeks, 12, 800 archtectures evaluated

[5] Barret Zoph and Quoc V Le (2016). “Neural architecture search with reinforcement learning”. In: *arXiv preprint arXiv:1611.01578*

Reinforcement learning

Reinforcement learning with a RNN controller

$$J(\theta_c) = E_{P(a_{1:T};\theta_c)}[R]$$

where R is the reward (e.g., accuracy on the validation dataset)

Apply REINFORCEMENT rule

$$\nabla_{\theta_c} J(\theta_c) = \sum_{t=1}^{T} E_{P(a_{1:T};\theta_c)}[\nabla_{\theta_c} \log P(a_t|a_{(t-1):1};\theta_c)R]$$

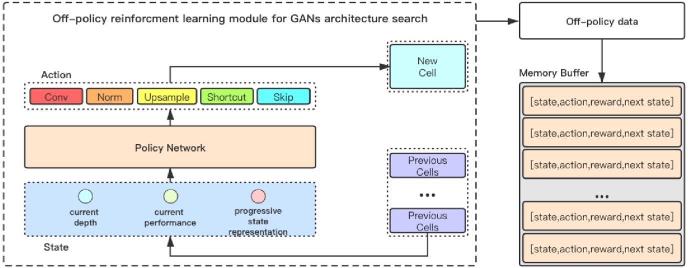
Use Monte Carlo approximation with control variate methods, the graident can be approximated by

Approximation of gradients

$$\frac{1}{m}\sum_{k=1}^{m}\sum_{t=1}^{T}\nabla_{\theta_c}\log P(a_t|a_{(t-1):1};\theta_c)(R_k - b)$$

Reinforcement Learning

Another example on GAN search: Yuan Tian et al. (2020). "Off-policy reinforcement learning for efficient and effective gan architecture search". In: *arXiv preprint arXiv:2007.09180*



Overview of the E^2GAN [6]

Reward define

$$R_t(s,a) = IS(t) - IS(t-1) + \alpha(FID(t-1) - FID(t))$$

The objective loss function

$$J(\pi) = \sum_{t=0} \mathbb{E}_{(s_t,a_t)\ p(\pi)} R(s_t,a_t) = \mathbb{E}_{architecture\ p(\pi)} IS_{final} - \alpha FID_{final}$$

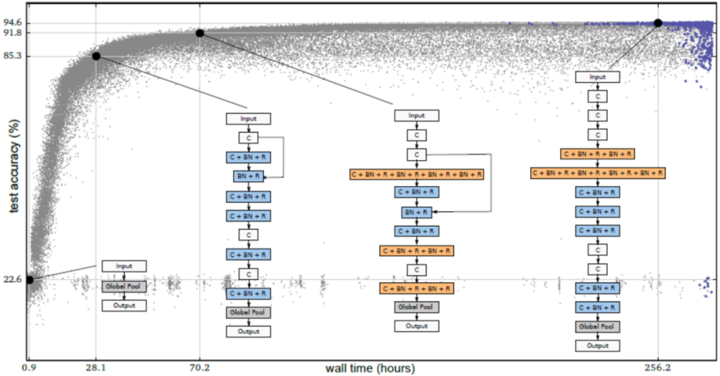
[6] Yuan Tian et al. (2020). "Off-policy reinforcement learning for efficient and effective gan architecture search". In: *arXiv preprint arXiv:2007.09180*

Evolution

Evolution methods

Neuroevolution (already since the 1990s)

- Typically optimized both architecture and weights with evolutionary methods
  e.g., Angeline, Saunders, and Pollack 1994; Stanley and Miikkulainen 2002
- Mutation steps, such as adding, changing or removing a layer
  e.g., Real, Moore, et al. 2017; Miikkulainen et al. 2017

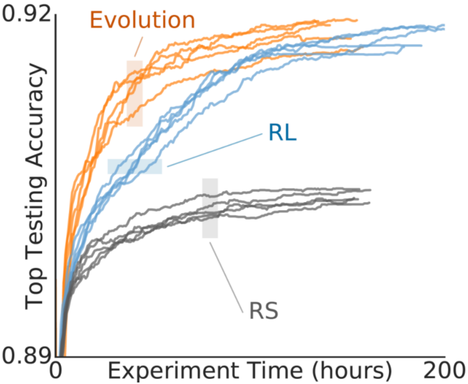


Regularized / Aging Evolution

Regularized / Aging Evolution methods

- Standard evolutionary algorithm e.g. Real, Aggarwal, et al. 2019
  But oldest solutions are dropped from the population (even the best)
- State-of-the-art results (CIFAR-10, ImageNet)
  Fixed-length cell search space

Comparison of evolution, RL and random search

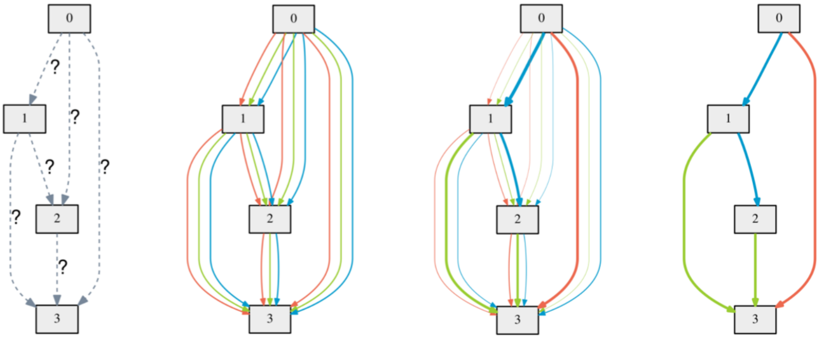


Baysian Optimization

Baysian optimzation methods

- Joint optimization of a vision architecture with 238 hyperparameters with TPE
  Bergstra, Yamins, and Cox 2013
- Auto-Net
  - Joint architecture and hyperparameter search with SMAC
  - First Auto-DL system to win a competition dataset against human experts
    Mendoza et al. 2016
- Kernels for GP-based NAS
  - Arc kernel
    Swersky, Snoek, and Adams 2013
  - NASBOT
    Kandasamy et al. 2018
- Sequential model-based optimization
  - PNAS
    C. Liu et al. 2018

DARTS



Overview of SNAS [7]

Continous relaxiation

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

[7] Hanxiao Liu, Karen Simonyan, and Yiming Yang (2018). "Darts: Differentiable architecture search". In: *arXiv preprint arXiv:1806.09055*

DARTS

A bi-level optimization

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

Algorithm 1 DARTS algorithm

Require: Create a mixed operation $\hat{O}^{(i,j)}$ parameterized by $\alpha^{(i,j)}$ for each edge (i, j)

Ensure: The architecture characterized by α

1: **while** not converged **do**

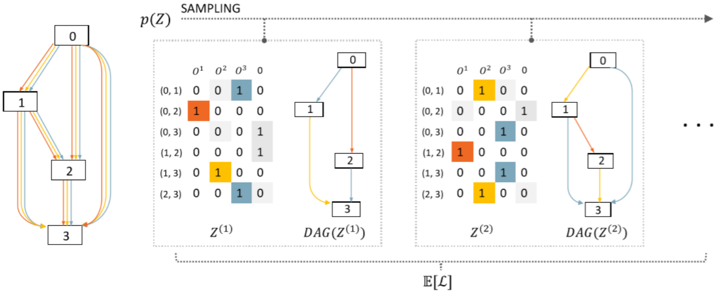
2: Update architecture α by descending $\nabla_\alpha \mathcal{L}_{val}(w - \xi \nabla_w \mathcal{L}_{train}(w, \alpha), \alpha)$
($\xi = 0$ if using first order approximation)

3: Update weights w by descending $\nabla_w \mathcal{L}_{train}(w, \alpha)$

4: **end while**

5: Derive the findal architecture based on the learned α

SNAS



Overview of SNAS [8]

Stochastic NAS

$$\mathbb{E}_{Z\ p_\alpha(Z)}[R(Z)] = \mathbb{E}_{Z\ p_\alpha(Z)}[L_\theta(Z)]$$
$$x_j = \sum_{i<j} \tilde{O}_{i,j}(x_i) = \sum_{i<j} Z_{i,j}^T O_{i,j}(x_i)$$

where $\mathbb{E}_{Z\ p_\alpha(Z)}[R(Z)]$ is the objective loss, $Z_{i,j}$ is a one-hot random variable vector to each edge (i,j) in the neural network and x_j is the intermediate node

[8] Sirui Xie et al. (2018). "SNAS: stochastic neural architecture search". In: *arXiv preprint arXiv:1812.09926*

SNAS

Apply Gummbel-softmax trick to relax the $p_\alpha(Z)$

$$Z_{i,j}^k = f_{\alpha_{i,j}}(G_{i,j}^k) = \frac{exp(\frac{(\log \alpha_{i,j}^k + G_{i,j}^k)}{\lambda})}{\sum_{l=0}^n exp(\frac{\log \alpha_{i,j}^l + G_{i,j}^l}{\lambda})}$$

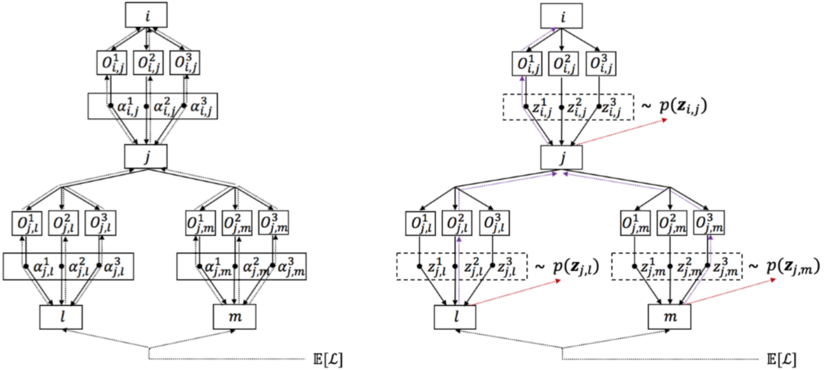
where $Z_{i,j}$ is the softened one-hot random variable, $\alpha_{i,j}$ is the architecture parameter, λ is the temperature of the Softmax function, and $G_{i,j}^k$ satisfies that

Gumbel distribution

$$G_{i,j}^k = -\log\left(-\log\left(U_{i,j}^k\right)\right)$$

where $U_{i,j}^k$ is a uniform random variable

Difference between DARTS and SNAS



A comparison between DARTS (i.e., the left) and SNAS (i.e., the right) [9]

Summary

- Deterministic gradients in DARTS and Stochastic gradients in SNAS
- DARTS require that the derived neural network should be retrained while SNAS has no need

[9] Sirui Xie et al. (2018). "SNAS: stochastic neural architecture search". In: *arXiv preprint arXiv:1812.09926*

Efficient methods

Main approaches for making NAS efficient

- Weight inheritance & network morphisms
- Weight sharing & one-shot models
- Discretize methods
- Multi-fidelity optimization
  Zela et al. 2018, Runge et al. 2018
- Meta-learning
  Wong et al. 2018

Network morphisms

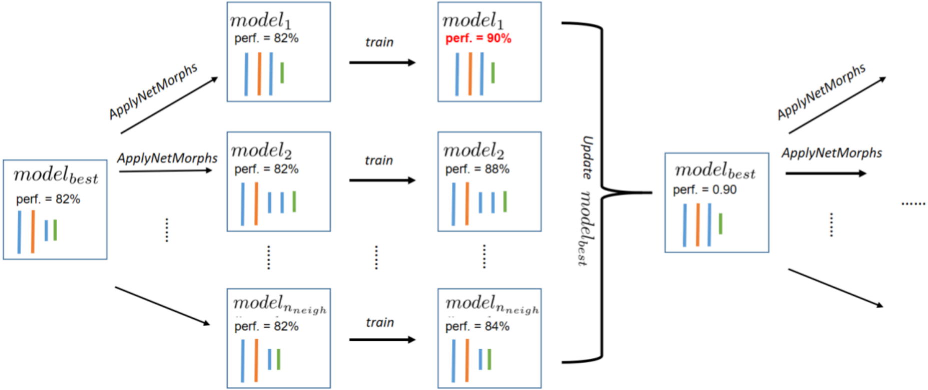
Network morphisms

Wei et al. 2016

- Change the network structure, but not the modelled function
  i.e., for every input the network yields the same output as before applying the network morphism
- Allow efficient moves in architecture space

Weight inheritance & network morphisms

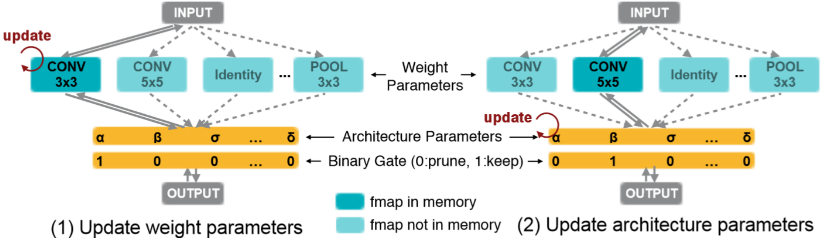
Cai, Chen, et al. 2017; Elsken, J. Metzen, and Hutter 2017; Cortes et al. 2017; Cai, J. Yang, et al. 2018



Discretize methods

Discretize the search space

Discretize the search space (e.g., operators, path, channels etc.) to achieve efficient NAS algorithms

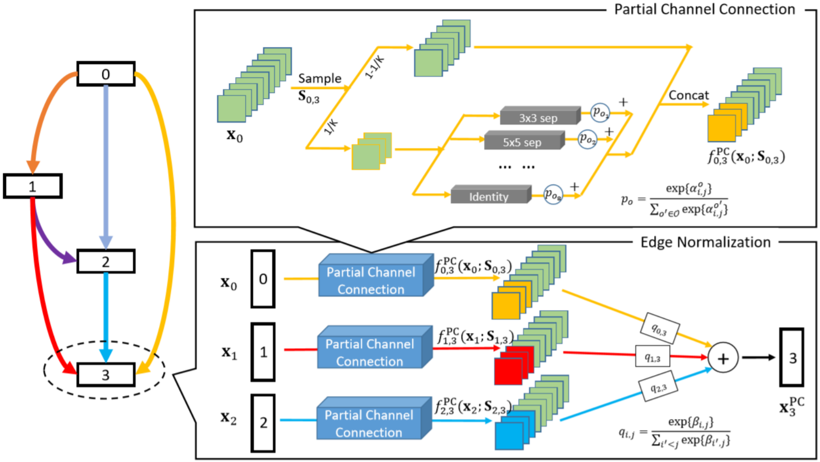


Learning both weight parameters and binarized architecture parameters [10]

[10] Han Cai, Ligeng Zhu, and Song Han (2018). "Proxylessnas: Direct neural architecture search on target task and hardware". In: *arXiv preprint arXiv:1812.00332*

Discretize methods

Another example: PC-DARTS



Overview of PC-DARTS. [11]

[11] Yuhui Xu et al. (2019). "Pc-darts: Partial channel connections for memory-efficient differentiable architecture search". In: *arXiv preprint arXiv:1907.05737*

Discretize methods

Partial channel connection

$$f_{i,j}^{PC}(x_i; S_{i,j}) = \sum_{o \in \mathcal{O}} \frac{exp\alpha_{i,j}^{o}}{\sum_{o' \in \mathcal{O}} exp\alpha_{i,j}^{o'}} \cdot (S_{i,j} * x_i) + (1 - S_{i,j} * x_i)$$

where $S_{i,j}$ defines a channel sampling mask, which assigns 1 to selected channels and 0 to masked ones.

Edge normalization

$$x_j^{PC} = \sum_{i<j} \frac{exp\beta_{i,j}}{\sum_{i'<j} exp\beta_{i',j}} \cdot f_{i,j}(x_i)$$

Edge normalization can mitigate the undesired fluctuation introduced by partial channel connection

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  - Differentiable search
  - Efficient methods
- NAS Benchmark
- Estimation strategy

Benchmark

The motivation

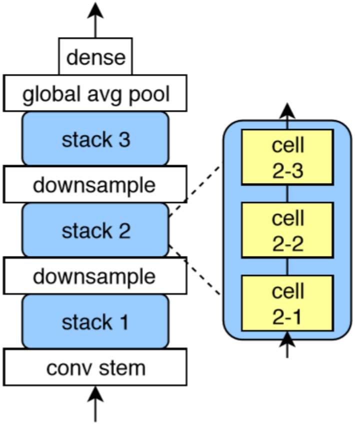
NAS algorithms are hard to reproduce normally

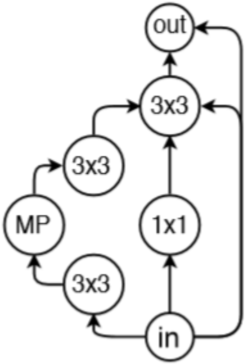
- Some NAS algorithms require months of compute time, making these methods inaccessible to most researchers
- Different proposed NAS algorithms are hard to compare since their different training procedures and different search spaces

Related works

- Chris Ying et al. (2019). "Nas-bench-101: Towards reproducible neural architecture search". In: *International Conference on Machine Learning*, pp. 7105–7114
- Xuanyi Dong and Yi Yang (2020). "Nas-bench-102: Extending the scope of reproducible neural architecture search". In: *arXiv preprint arXiv:2001.00326*

NAS-Bench-101





Operation on node

The stem of the search space

The stem is composed of three cells, followed by a downsampling layer. The downsampling layer halves the height and width of the feature map via max-pooling and the channel count is doubled. The pattern are repeated three times, followed by global average pooling and a final dense softmax layer. The initial layer is a stem consisting of one 3×3 convolution with 128 output channels.

NAS-Bench-101

The space of cell architectures is a directed acyclic graph on V nodes and E edges, each node has one of L labels, representing the corresponding operation. The constraints on the search space

The search space

- $L = 3$
  - 3×3 convolution
  - 1×1 convolution
  - 3×3 max-pool
- $V \leq 7$
- $E \leq 9$
- input node and output node are pre-defined on two of V nodes

Encoding is implemented as a 7×7 upper-triangular binary matrix, by de-duplication and verification, there are **423, 000** neural network architectures

NAS-Bench-101

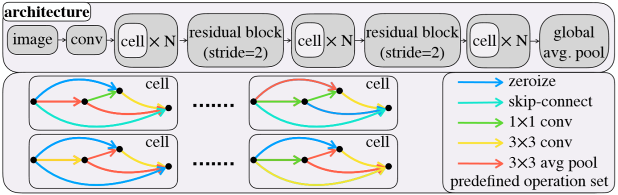
The dataset of NAS-Bench-101 is a mapping from the $(A, Epoch, trial\#)$ to

- Training accuracy
- Validation accuracy
- Testing accuracy
- Training time in seconds
- Number of trainable parameters

Applications

- Compare different NAS algorithms
- Research on generalization abilities of NAS algorithms

NAS-Bench-201



Top: the macro skeleton of each architecture candidate. **Bottom-left**: examples of neural cell with 4 nodes. Each cell is a directed acyclic graph, where each edge is associated with an operation selected from a predefined operation as shown in **Bottom-right**

Comparison between NAS-Bench-101 and NAS-Bench-201

NAS-Bench-101 uses Operation on node while NAS-Bench-201 uses Operation on edge as its search space

	#architectures	#datasets	$\|\mathcal{O}\|$	Search space constraint	Supported NAS alogrithms	Diagnostic information
NAS-Bench-101	510M	1	3	constrain #edges	partial	-
Nas-Bench-201	15.6K	3	5	no constraint	all	fine-grained info. (e.g., #params, FLOPs, latency)

Overview

Estimation strategy

Strategy

- Task specific
  - Classficiation tasks
    e.g., accuracy, error rate, etc.
  - Segmentation tasks
    e.g., pixel accuracy, MIoU
  - Generation tasks
    e.g., Inception Score, Frechet Inception Score, etc.
- Latency considered factors
  - #FLOPs
  - #Parameters

Tips

Different NAS methods can incorporate diverse factors into search consideration