AutoML: Neural Architecture Search

Part 1: Introduction and Black-box Approaches

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Overview

Neural Architecture Search (NAS)

- Goal: automatically find neural architectures with strong performance
  - Optionally, subject to a resource constraint

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images/NAS-papers.png

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- One of the main problems AutoML is known for

- Initially extremely expensive
- By now several methods promise low overhead over a single model training

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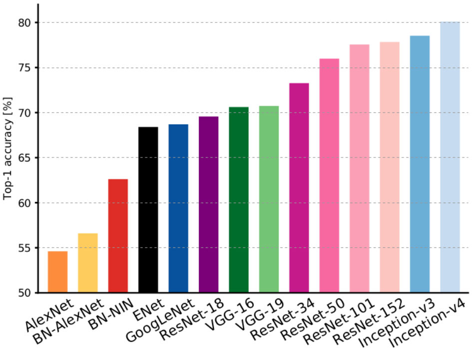
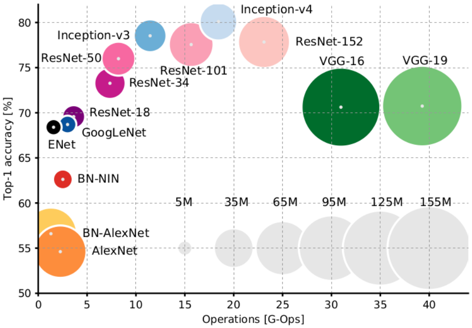
Motivation for NAS

- Performance improvements on various tasks due to novel architectures
- Can we automate this design process, potentially discovering new components/topologies?

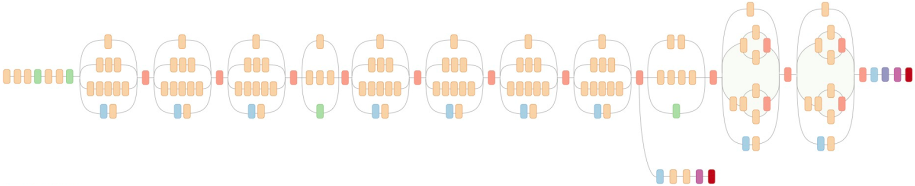




[Canziani et al. 2017]

Motivation for NAS

- Manual design of architectures is time consuming
- Complex state-of-the-art architectures are a result of years of trial and errors by experts



Inception-v3 [Szegedy et al. 2016]

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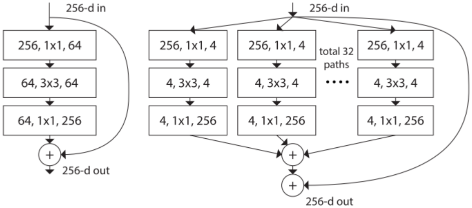
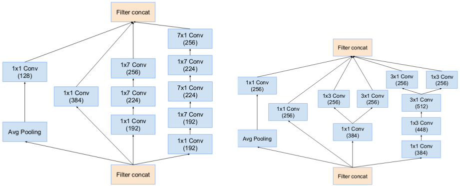
- Manual design of architectures is time consuming
- Complex state-of-the-art architectures are a result of years of trial and errors by experts
    - Main pattern: Repeated blocks with same structure (topology)

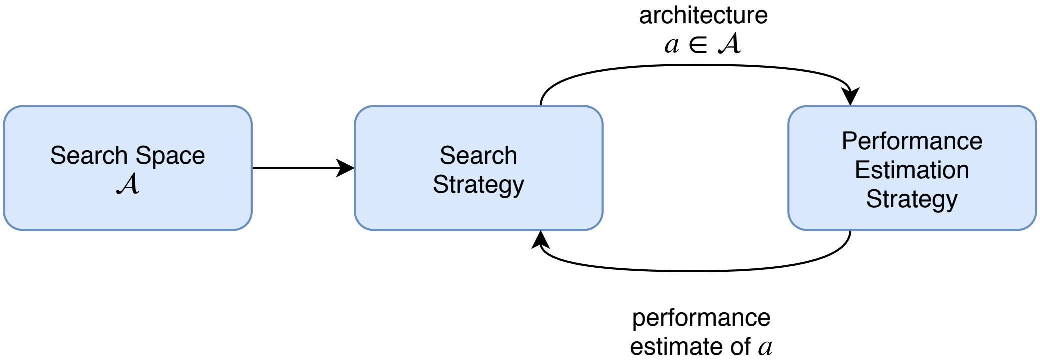


ResNet/ResNeXt blocks
[He et al. 2016; Xie et al. 2016]



Inception-v4 blocks [Szegedy et al. 2017]

NAS components [Elsken et al. 2019]



- Search Space: the types of architectures we consider; micro, macro, hierarchical, etc.
- Search Strategy: Reinforcement learning, evolutionary strategies, Bayesian optimization, gradient-based, etc.
- Performance Estimation Strategy: validation performance, lower fidelity estimates, one-shot model performance, etc.

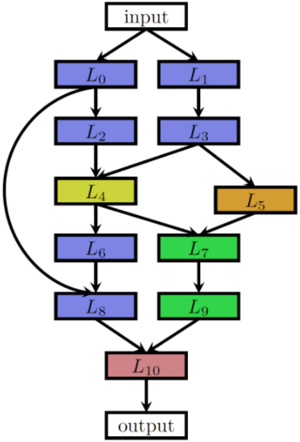
Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  List three major components of NAS methods.
- Discussion:
  Is there a problem for which you would like to apply NAS yourself?

Search Spaces

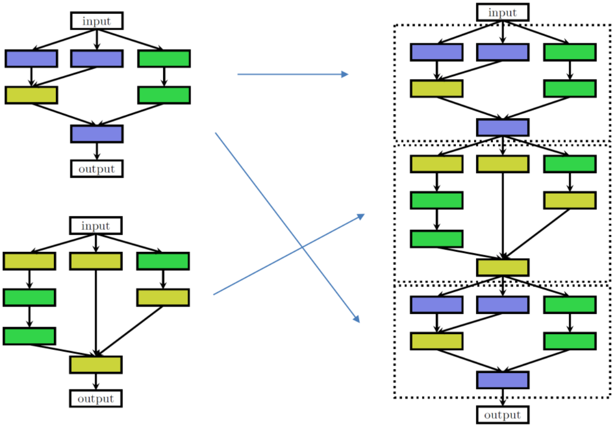
Basic Neural Architecture Search Spaces

Chain-structured space
(different colours:
different layer types)



More complex space
with multiple branches
and skip connections

Cell Search Spaces [Zoph et al., 2018]



Two possible cells

Architecture composed of stacking together individual cells

Details on Cell Search Spaces [Zoph et al., 2018]

- 2 types of cells: normal and reduction cells
- For each type of cell: B blocks, each with 5 choices
  - Choose two previous feature maps (from this cell)
  - For each of these, choose an operation (3×3 conv, max-pool, etc.)
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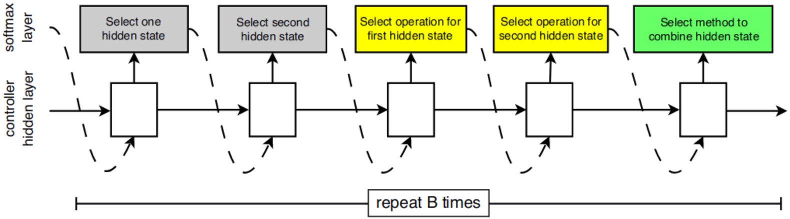
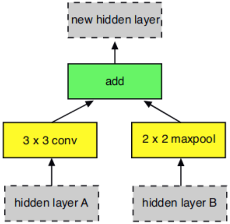
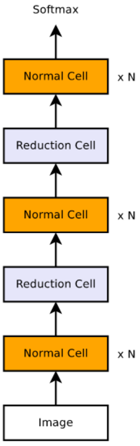
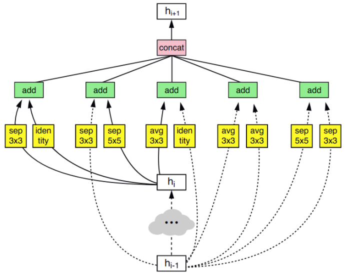




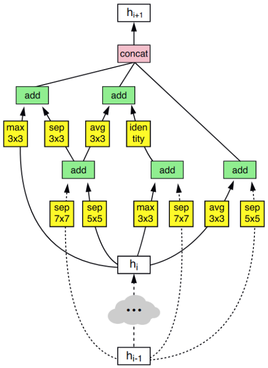
Example of an architecture sample with B=5



CIFAR10
Architecture



Normal Cell



Reduction Cell

Source: [Zoph et al., 2018]

Pros and Cons of Cell Search Space

What are some pros and cons of the cell search space compared to the basic one?

Please think about this for a few minutes before continuing.

Pros and Cons of Cell Search Space

Pros:

- Reduced search space size; speed-ups in terms of search time.
- Transferability to other datasets (e.g., cells found on CIFAR-10 transfer to ImageNet)
- Stacking repeating patterns is proven to be a useful design principle (ResNet, Inception, etc.)

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Cons:

- Still need to (manually) determine the *macro* architecture, i.e., the way in which cells are connected.
- Limiting if different cells work better in different parts of the network
  - E.g., different spatial resolutions may favour different convolutions

Hierarchical representation of search space [Liu et al, 2017]

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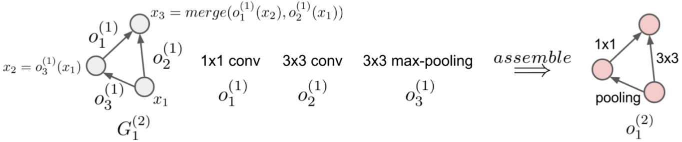

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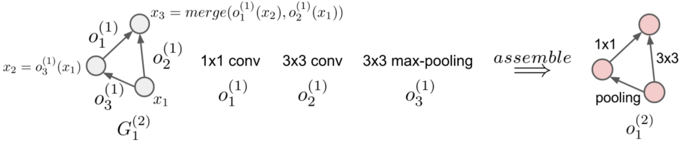
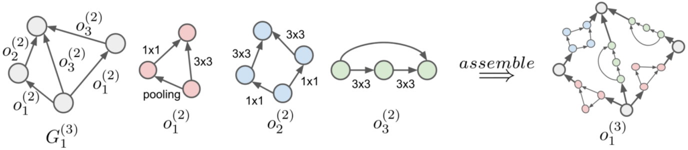


  - Level-3 motivs: combinations of level-2 motivs



Pros and Cons of Hierarchical Search Space

What are some pros and cons of a hierarchical search space compared to the cell search space?

Please think about this for a few minutes before continuing.

Pros and Cons of Hierarchical Search Space

Pros:

- Flexibility of constructing building blocks and reusing them many times
  - like a cell search space
- Flexibility of using different building blocks in different parts of the network
  - like a basic search space
- Ability to reuse building blocks at various levels of abstraction
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Cons:

- Larger than cell search space
- Vastly more expressive than cell search space $\rightarrow$ potentially much harder to search

Questions to Answer for Yourself / Discuss with Friends

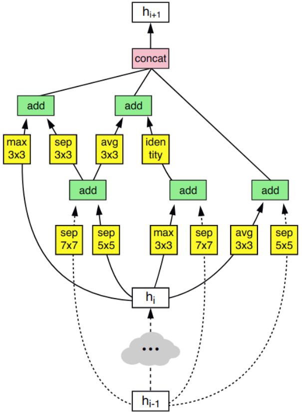
- Repetition:
  What are some pros and cons of the cell search space compared to the basic one?
- Repetition:
  Explain the way in which level-3 motivs in the hierarchical search space use level-2 motivs.
- Repetition:
  What are some pros and cons of the hierarchical search space compared to the other ones?

Blackbox Optimization Methods

NAS as Hyperparameter Optimization

- NAS can be formulated as a HPO problem

- E.g., cell search space by [Zoph et al. 2018] has 5 categorical choices per block
  - 2 categorical choices of hidden states
    - For block N, the domain of these categorical variables is $\{h_i, h_{i-1}, \text{output of block } 1, \ldots, \text{output of block } N-1\}$
  - 2 categorical variables choosing between operations
  - 1 categorical variable choosing the combination method
  - Total number of hyperparameters for the cell: 5B (with B=5 by default)



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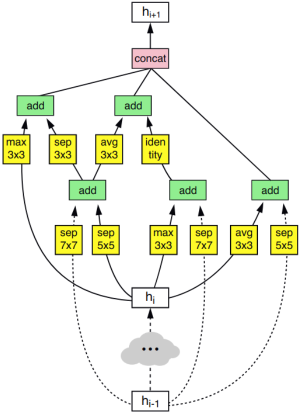

Reduction Cell

- In general: one may require conditional hyperparameters
  - E.g., chain-structured search space
    - ★ Top-level hyperparameter: number of layers L
    - ★ Hyperparameters of layer k conditional on L $\geq$ k

Early NAS Methods

- Neuroevolution (already since the 1990s) [Kitano 1990; Angeline et al. 1994; Stanley and Miikkulainen, 2002; Bayer et al, 2009; Floreano et al. 2008]
  - Evolves architectures & often also their weights
  - Typical approach:
    - Initialize a population of N random architectures
    - Sample N individuals from that population (with replacement) according to their fitness
    - Apply mutations to those N individuals to produce the next generation's population
  - Mutations include adding, changing or removing a layer

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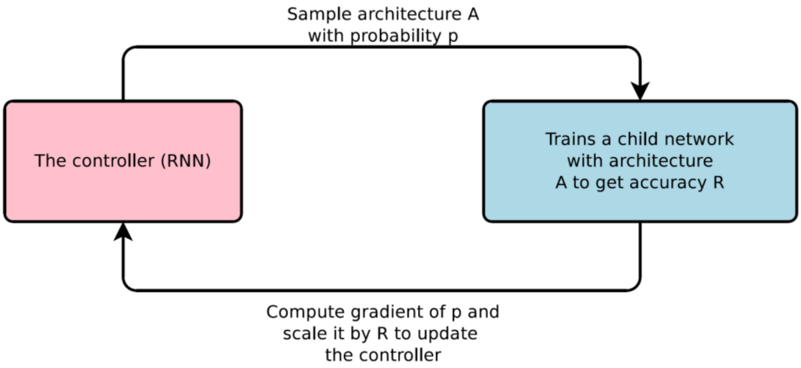
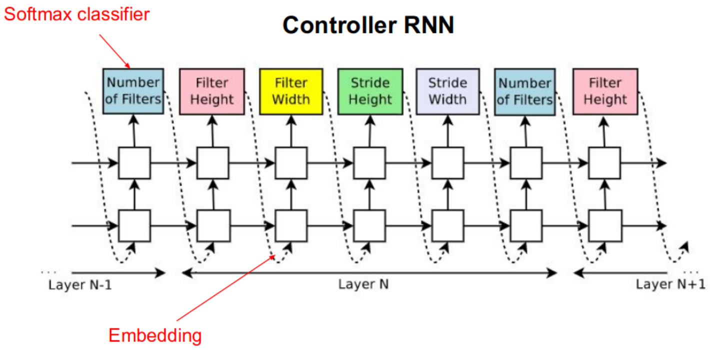
- Bayesian optimization (since 2013)
  - With TPE:
    - ⋆ Joint optimization of a vision architecture with 238 hyperparameters [Bergstra et al, 2013]
  - With SMAC: joint architecture and hyperparameter search, yielding
    - ⋆ New state-of-the-art performance on CIFAR-10 w/o data augmentation [Domhan et al. 2015]
    - ⋆ First Auto-DL system to win competition dataset against human experts [Mendoza et al. 2016]
  - With Gaussian processes:
    - ⋆ Arc kernel [Swersky et al, 2013]

Reinforcement Learning [Zoph & Le, 2017]



- Use RNN ("Controller") to generate a NN architecture piece-by-piece
- Train this NN ("Child Network") and evaluate it on a validation set
- Use Reinforcement Learning (RL) to update the parameters of the Controller RNN to optimize the performance of the child models

Learning CNNs with RL [Zoph & Le, 2017]



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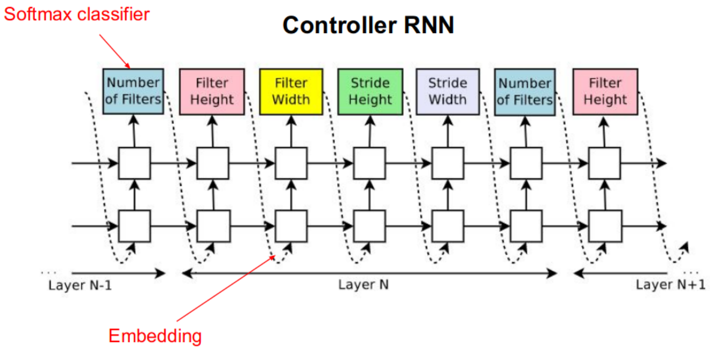

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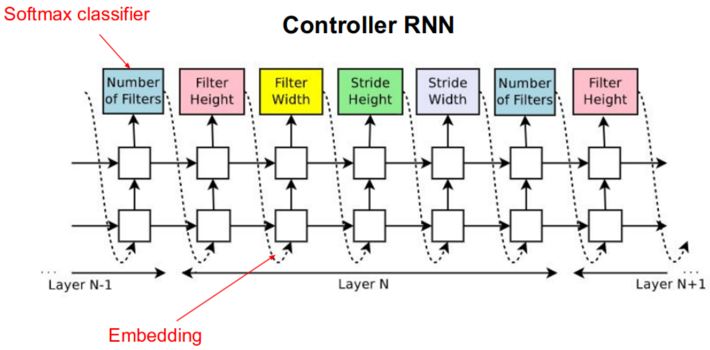

- For a fixed number of layers, select:
  - Filter width/height, stride width/height, number of filters
- Large computational demands (800 GPUs for 2 weeks, 12.800 architectures evaluated)
- State-of-the-art results for CIFAR-10 & Penn Treebank architecture

  $\rightarrow$ Brought NAS into the limelight

Learning CNN cells with RL [Zoph et al. 2018]

- 2 types of cells: normal and reduction cells
- For each type of cell: B blocks, each with 5 choices
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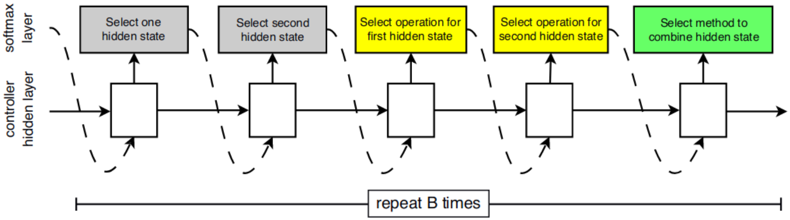

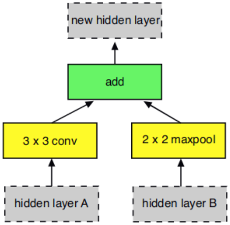

Learning CNN cells with evolution [Real et al, 2019]

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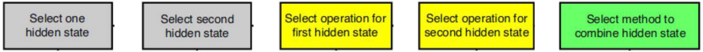
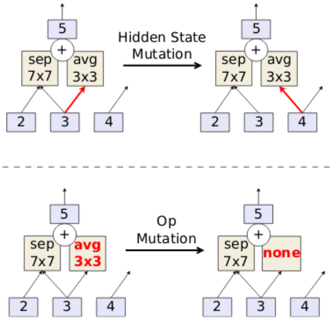
- Evolution simply tackles this as a HPO problem with 2×5×B variables:



Regularized/Aging Evolution [Real et al, 2019]

- Quite standard evolutionary algorithm
  - But oldest solutions are dropped from population, instead of the worst
- Standard SGD for training weights (optimizing the same blackbox as RL)
- Same fixed-length (HPO) search space as used for RL [Zoph et al. 2018]



Different types of mutations in cell search space

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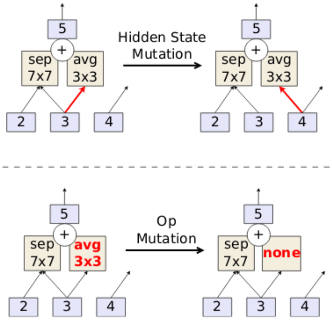

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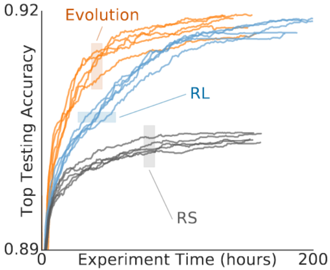

State-of-the-art performance in apples-to-apples comparison → AmoebaNet

Bayesian Optimization (BO)

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- Auto-Net [Mendoza et al. 2016]
  - Using BO with a random forest model (SMAC [Hutter et al, 2011])
  - Already won several datasets against human experts
    - E.g., human action recognition data set in 2015: 54491 data points, 5000 features, 18 classes
    - First automated deep learning (Auto-DL) method to win a machine learning competition dataset against human experts

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- Kernels for GP-based NAS
  - Arc kernel [Swersky et al, 2013]
  - NASBOT [Kandasamy et al, 2018]
- There are also several recent promising BO approaches based on neural networks
  - BANANAS [White et al. 2020]

Current State of the Art: Differential Evolution

- Comprehensive experiments on a wide range of 12 different NAS benchmarks
  [Awad, Mallik and Hutter, AutoML 2020]
- Results:
  - Regularized evolution is very robust, typically amongst best of the methods discussed so far
  - Evolution variant of differential evolution is yet better; most efficient and robust method

Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  What are some pros and cons of using black-box optimizers for NAS?
- Repetition:
  How can NAS be modelled as a HPO problem?
- Discussion:
  Given enough resources, will blackbox NAS approaches always improve performance?
- Discussion:
  Why does discarding the oldest individual (rather than the worst) help in regularized/aging evolution?
- Transfer:
  How would you write NAS with the hierarchical search space as a HPO problem?

Speedup Techniques

Overview of NAS Speedup Methods

- Multi-fidelity optimization
- Learning curve prediction
- Meta-learning across datasets
- Network morphisms & weight inheritance
- Weight sharing & the one-shot model

NAS Speedup Technique 1: Multi-fidelity optimization

- Analogous to multi-fidelity optimization in HPO
  - Many evaluations for cheaper fidelities (less epochs, smaller datasets, down-sampled images, shallower networks, etc)
  - Fewer evaluations necessary for more expensive fidelities

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  - Fewer evaluations necessary for more expensive fidelities
- Compatible with any blackbox optimization method
  - Using random search: ASHA [Li & Talwalkar, 2019]
  - Using Bayesian optimization: BOHB [Zela et al, 2018]
  - Using differential evolution: DEHB [Awad et al, under review]
  - Using regularized evolution: progressive dynamic hurdles [So et al, 2019]

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  - Using regularized evolution: progressive dynamic hurdles [So et al, 2019]
- Often used for joint optimization of architecture & hyperparameters
  - Auto-Pytorch [Mendoza et al, 2019] [Zimmer et al, under review]
  - "Auto-RL" [Runge et al, 2019]

NAS Speedup Technique 2: Learning Curve Prediction

- Analogous to learning curve prediction in HPO
  - Observe initial learning curve and predict performance at the end
  - Can use features of the architecture as input (just like hyperparameters as inputs)

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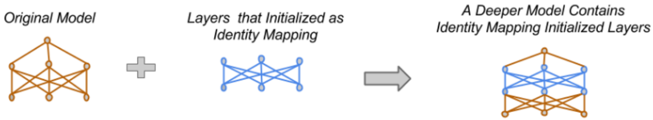
- Compatible with any blackbox optimization method
  - Using random search and Bayesian optimization: [Domhan et al, 2015]
  - Using reinforcement learning: [Baker et al, 2018]

NAS Speedup Technique 3: Meta-Learning

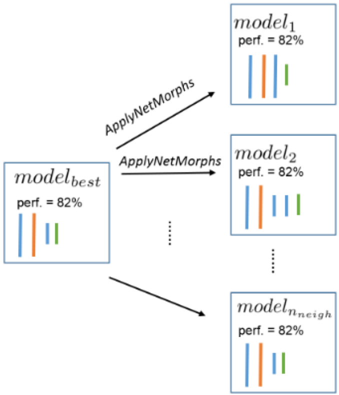
- Lots of work on meta-learning for HPO
- Only little work on meta-learning for NAS
  - Learn RL agent's policy network on previous datasets [Wong et al, 2018]
  - Learn neural architecture that can be quickly adapted [Lian et al, 2019; Elsken et al, 2019]
  - Find a set of good architectures to initialize BOHB in Auto-Pytorch [Zimmer et al, under review]

NAS Speedup Technique 4: Network Morphisms

- Network Morphisms [Chen et al. '16; Wei et al. '16; Cai et al. '17]
  - Change the network structure, but not the modelled function
  - i.e., for every input the network yields the same output as before applying some network morphisms operations, such as "Net2DeeperNet", "Net2WiderNet", etc.



Network Morphisms Allow Efficient Moves in Architecture Space



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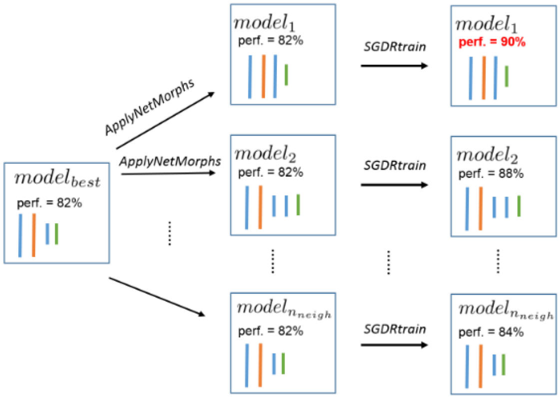

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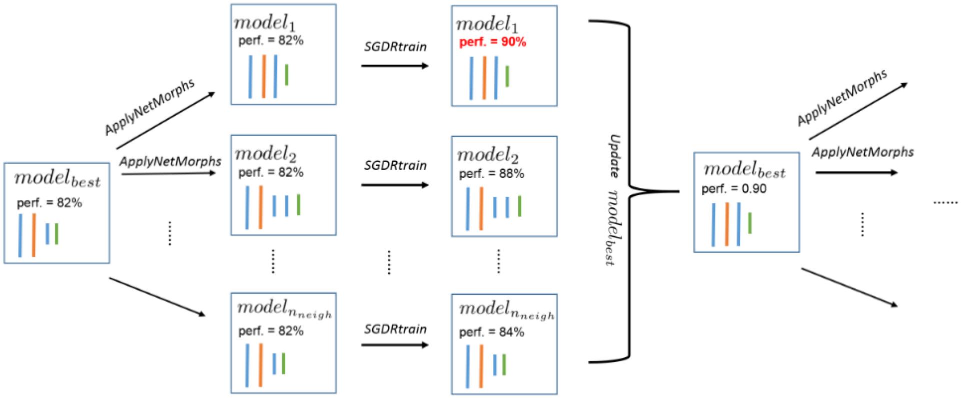

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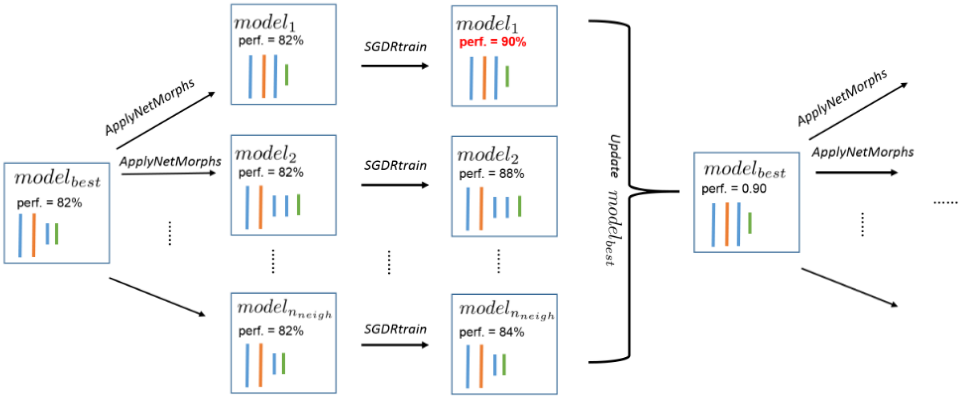


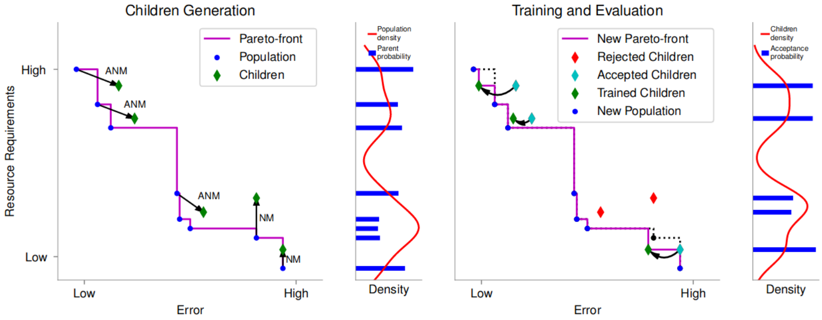
Weight inheritance avoids expensive retraining from scratch

[Real et al, 2017, Cai et al, 2018, Elsken et al, 2017, Cortes et al, 2017, Cai et al, 2018, Elsken et al. '19]

Network Morphisms for Multi-objective NAS [Elsken et al. '19]

LEMONADE: Lamarckian Evolution for Multi-Objective Neural Arch. Design

- Maintain a Pareto front of the 2 or more objectives
  - Evolve a population of Pareto-optimal architectures over time
  - "Lamarckian": children inherit the weights of the parent's architecture



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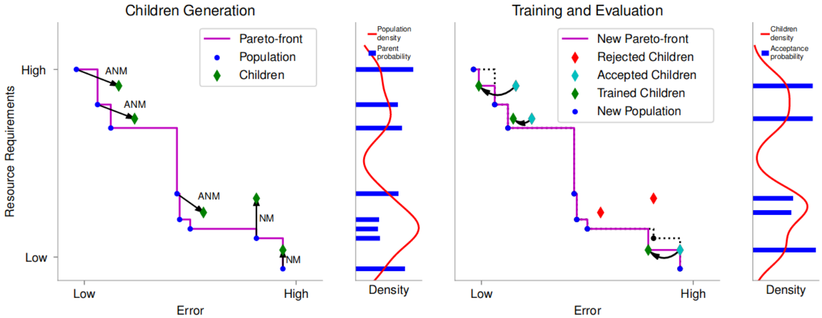
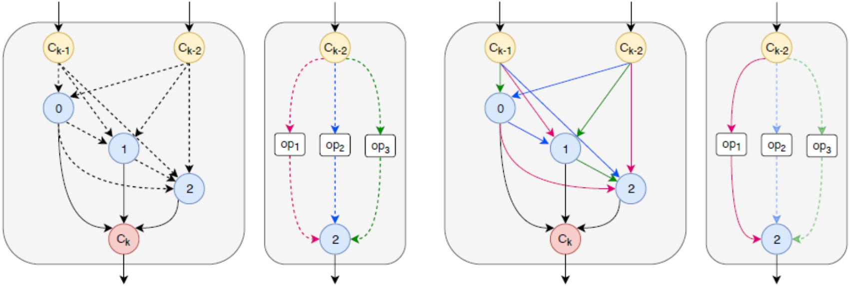


- Also include operators to shrink the network
  - Dropping layers, dropping units within a layer, etc.
  - Use approximate network morphisms (function not preserved perfectly)

NAS Speedup Technique 5: Weight Sharing and One-shot Models [Pham et al, 2018; Bender et al, 2018]

- DAG (Multigraph) representation
  - ⇒ Nodes - latent representations.
  - ⇒ Edges (dashed) - operations.
- Architecture optimization problem: Find optimal path from the input to the output



(a) One-shot search **(b)** Final evaluation

NAS Speedup Technique 5: Weight Sharing and One-shot Models [Pham et al, 2018; Bender et al, 2018]

- All possible architectures are subgraphs of a large supergraph: the one-shot model
- Weights are shared between different architectures with common edges/nodes in the supergraph
- Search costs are reduced drastically since one only has to train a single model (the one-shot model).

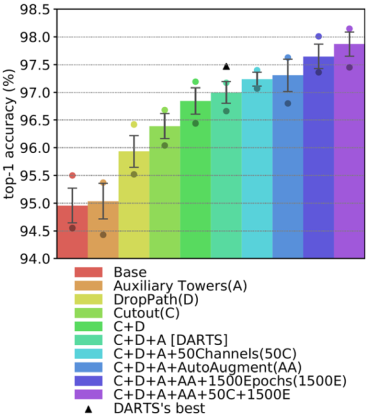
Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  List five methods to speed up NAS over blackbox approaches
- Repetition:
  Which speedup techniques directly carry over from HPO to NAS?
- Discussion:
  Why do network morphisms and the one-shot model only apply to NAS, and not to HPO?

Issues and Best Practices in NAS Research

Issues in NAS Research & Evaluations

- Most NAS methods are extremely difficult to reproduce and compare [Li & Talwalkar, 2019]
- For benchmarks used in almost all NAS papers:
  - Training pipeline matters much more than neural architecture



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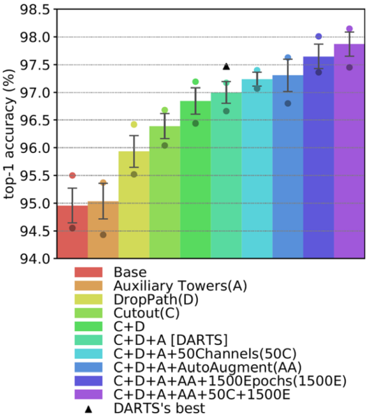

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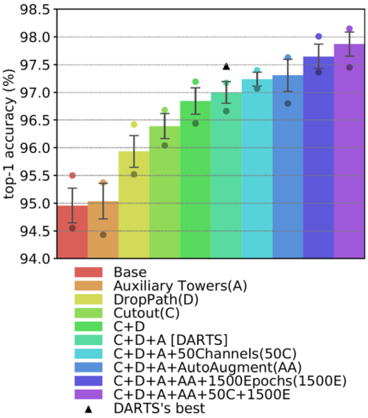
→ We emphasize concepts, not published performance numbers



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Building a Scientific Community for NAS

- Benchmarks
  - NAS-Bench-101 [Ying et al, ICML 2019]
  - NAS-Bench-201 [Dong et al, ICML 2020]
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- First NAS workshop at ICLR 2020

Best Practice Checklist for NAS Research [Lindauer & Hutter, 2020]

- Best practices for releasing code
  - Code for the training pipeline used to evaluate the final architectures
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- Note that the easiest way to satisfy the first three is to use existing NAS benchmarks

Definition: NAS Benchmark [Lindauer & Hutter, 2020]

A NAS benchmark consists of a dataset (with a predifiend training-test split), a search space, and available runnable code with pre-defined hyperparameters for training the architectures.

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  - Did you perform multiple runs of your experiments and report seeds?
  - Did you use tabular or surrogate benchmarks for in-depth evaluations?

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- We believe the community would benefit a lot from:
  - Clean NAS benchmarks for new applications
    - Including all details for the application. No need to also develop a new method.
  - Open-source library of NAS methods to compare methods without confounding factors
    - First version already developed: NASlib [Zela et al, under review]

NAS-Bench-101: The First NAS Benchmark [Ying et al, 2018]

- Dataset: CIFAR-10, with the standard training/test split
- Runnable open-source code provided in Tensorflow
- Cell-structured search space consisting of all directed acyclic graphs (DAGs) on V nodes, where each possible node has L operation choices.

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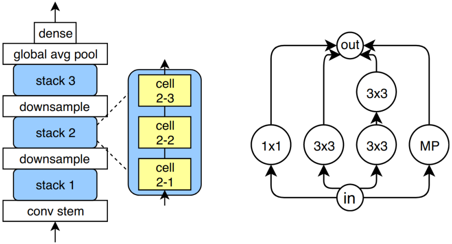
- To limit the number of architectures, NAS-Bench-101 has the following constraints:
  - $L = 3$ operators:
    - 3×3 convolution
    - 1×1 convolution
    - 3×3 max-pooling
  - $V \leq 7$ nodes
  - A maximum of 9 edges



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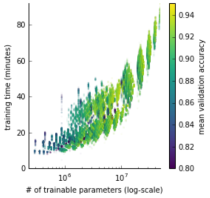
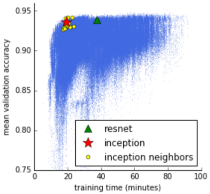
- Around 423k unique cells
  - 4 epoch budgets: 4, 12, 36, 108
  - 3 repeats
  - around 5M trained and evaluated models
  - 120 TPU years of computation
  - the best architecture mean test accuracy: 94.32%





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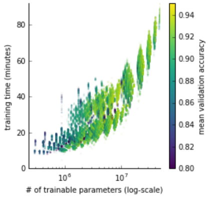
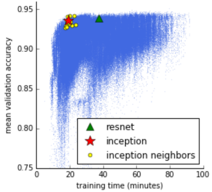
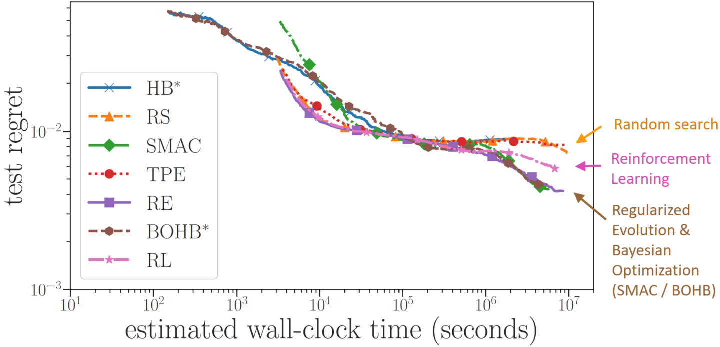


- Given an architecture encoding A, budget E_{stop} and trial number, one can query from NAS-Bench-101 the following quantities:
  - training/validation/test accuracy
  - training time in seconds
  - number of trainable model parameters



Evaluation of Blackbox NAS Methods on NAS-Bench-101 [Ying et al, 2019]

- RL outperforms random search
- BO and regularized evolution perform best, better than RL



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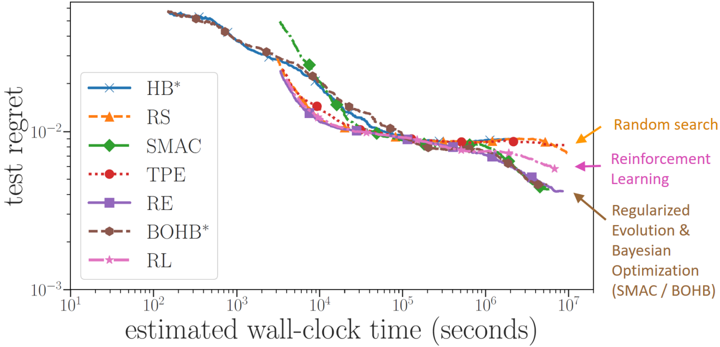

- Note that the BO method SMAC [Hutter et al, 2011] predated RL for NAS [Zoph & Le, 2017] by 6 years
  - Only now, benchmarks like NAS-Bench-101 allow for efficient comparisons

Questions to Answer for Yourself / Discuss with Friends

- Repetition:
  For the most common NAS search space, how important is the NAS component compared to the importance of the training pipeline used?

- Repetition:
  Why do we need proper benchmarking of NAS algorithms?

- Repetition:
  What does a NAS benchmark consist of?

- Repetition:
  List all best practices for NAS you remember.