Neural Architecture Search: Foundations and Trends

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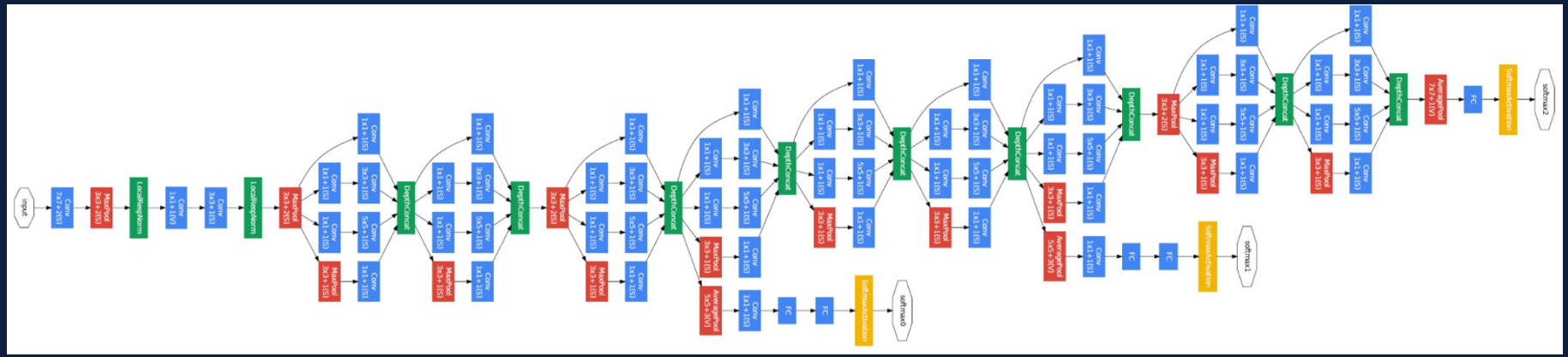
Slides (with hyperlinks): https://crwhite.ml/

Machine learning: a story of automation

```
from torchvision.models import resnet50, ResNet50_Weights

# Best available weights (currently alias for IMAGENET1K_V2)
# Note that these weights may change across versions
resnet50(weights=ResNet50_Weights.DEFAULT)
```

Neural architecture search

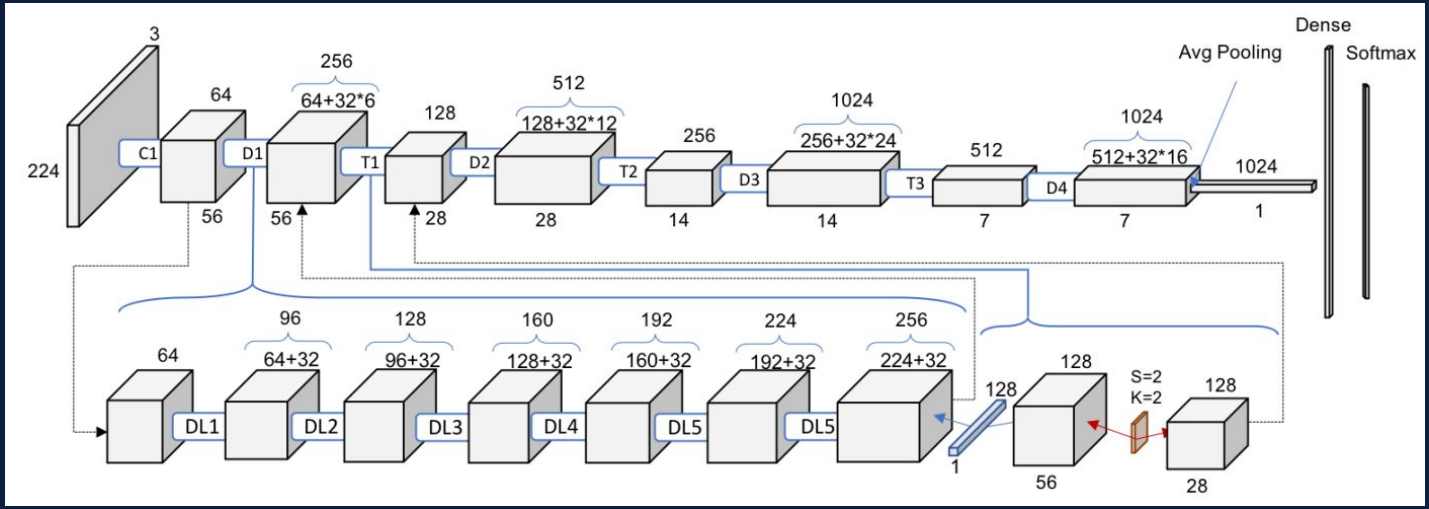


GoogLeNet (2014)

Architectures are getting increasingly more specialized and complex

Source: GoogLeNet (2014)

Neural architecture search

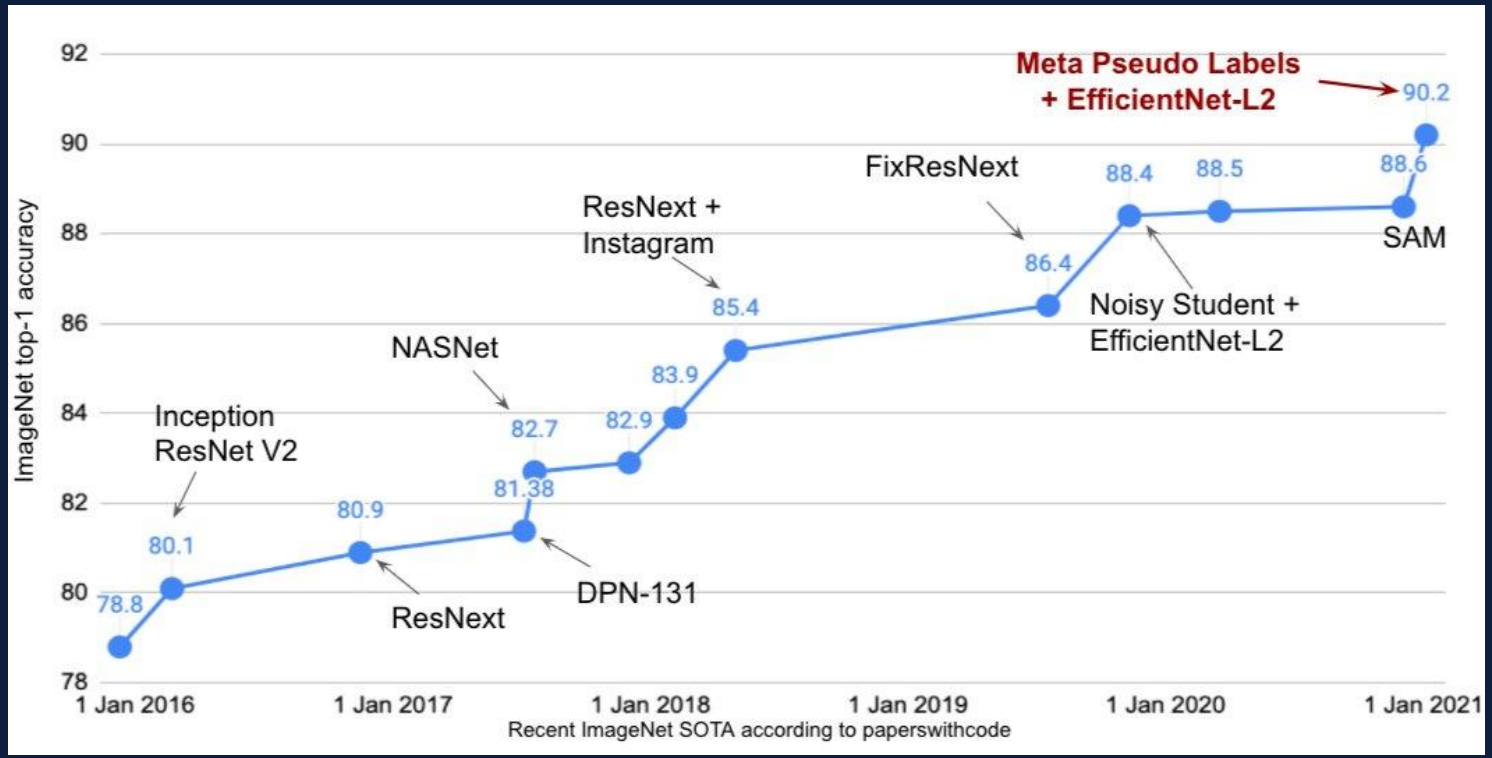


DenseNet (2016)

Architectures are getting increasingly more specialized and complex

Source: DenseNet (2016)

Neural architecture search



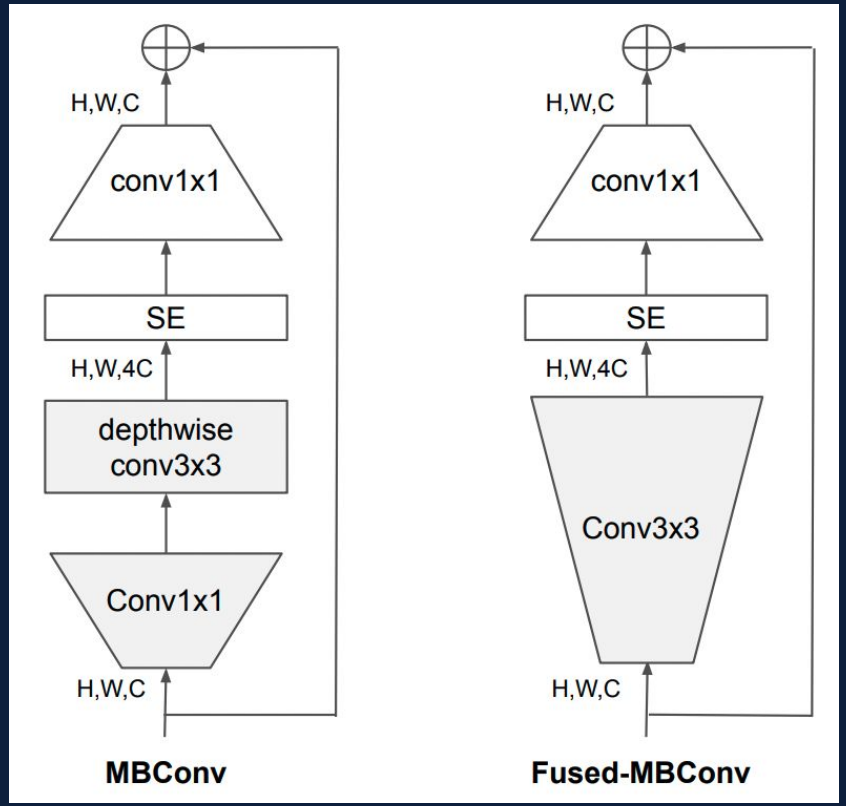
Searched models are replacing **human-designed** models

Source: https://twitter.com/quocleix/status/1349443438698143744/

Human + Neural architecture search

Stage i	Operator $\hat{\mathcal{F}}_i$	Resolution $\hat{H}_i \times \hat{W}_i$	#Channels $\hat{C}_i$	#Layers $\hat{L}_i$
1	Conv3x3	224×224	32	1
2	MBConv1, k3x3	112×112	16	1
3	MBConv6, k3x3	112×112	24	2
4	MBConv6, k5x5	56×56	40	2
5	MBConv6, k3x3	28×28	80	3
6	MBConv6, k5x5	14×14	112	3
7	MBConv6, k5x5	14×14	192	4
8	MBConv6, k3x3	7×7	320	1
9	Conv1x1 & Pooling & FC	7×7	1280	1

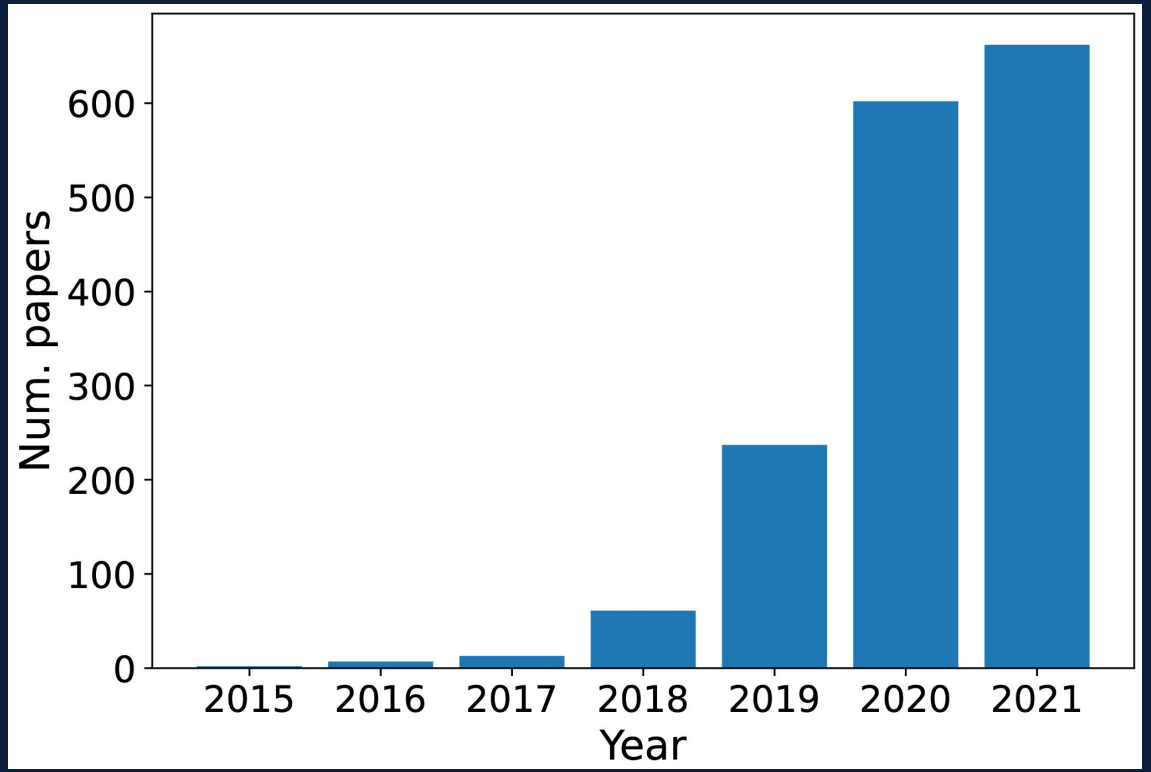
Stage	Operator	Stride	#Channels	#Layers
0	Conv3x3	2	24	1
1	Fused-MBConv1, k3x3	1	24	2
2	Fused-MBConv4, k3x3	2	48	4
3	Fused-MBConv4, k3x3	2	64	4
4	MBConv4, k3x3, SE0.25	2	128	6
5	MBConv6, k3x3, SE0.25	1	160	9
6	MBConv6, k3x3, SE0.25	2	256	15
7	Conv1x1 & Pooling & FC	-	1280	1



Source: EfficientNet (2019), EfficientNetV2 (2021)

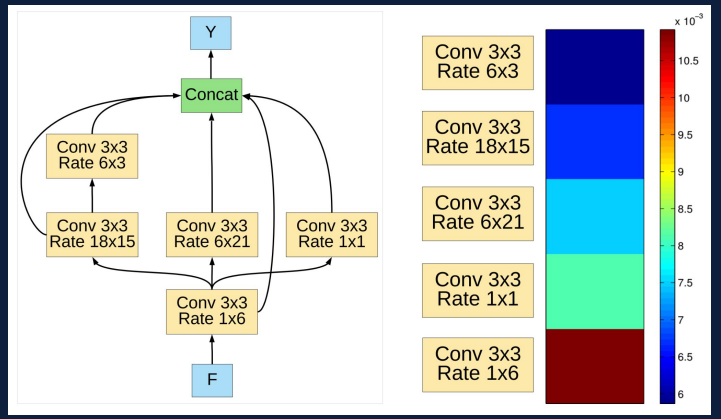
Neural architecture search

NAS: the process of **automating** the design of **neural architectures** for a given dataset.



New Datasets

Spherical	Omnidirectional Vision	
NinaPro DB5	Prosthetics Control	
FSD50K	Audio Classification	
Darcy Flow	PDE Solver	
PSICOV	Protein Folding	
Cosmic	Astronomy Imaging	
ECG	Medical Diagnostics	
Satellite	Earth Monitoring	
DeepSEA	Genetic Prediction	

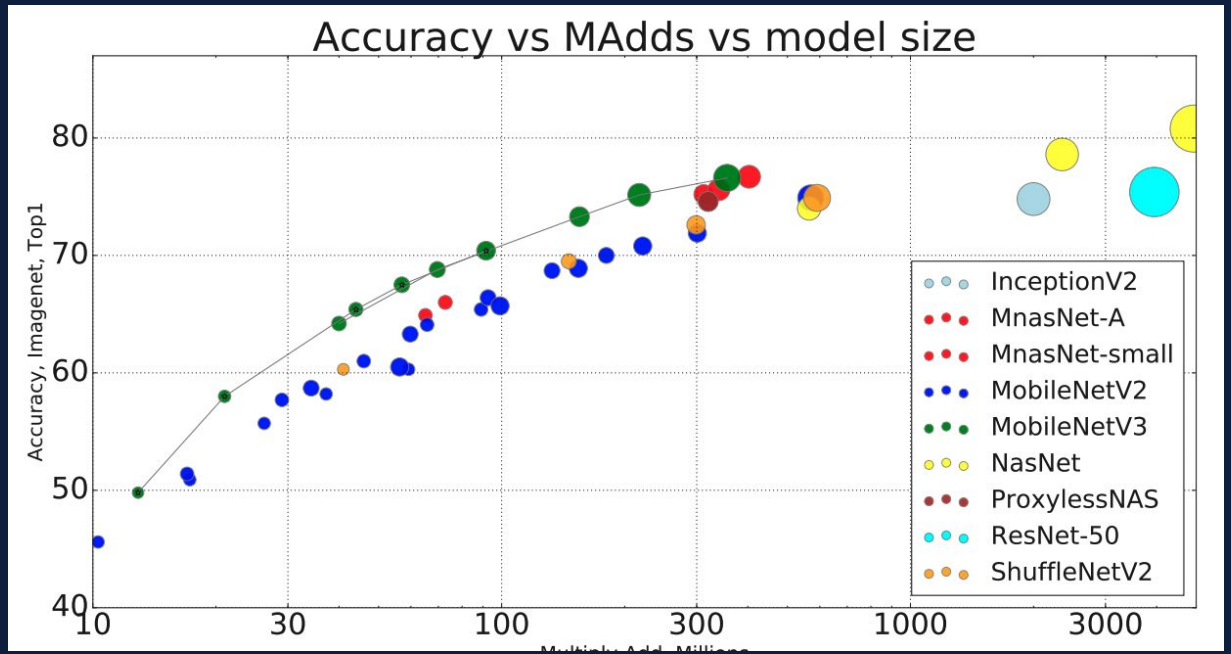


Graph neural networks . . . . .
Generative adversarial network
Dense prediction tasks . . . . .
Adversarial robustness . . . . .
Self-supervised learning for NAS

Source: NAS-Bench-360 (2021)

Chen et al. 2018

Fitting Models on Edge Devices



Input	Operator	exp size	#out	SE	NL	s
$224^2 \times 3$	conv2d	-	16	-	HS	2
$112^2 \times 16$	bneck, 3x3	16	16	-	RE	1
$112^2 \times 16$	bneck, 3x3	64	24	-	RE	2
$56^2 \times 24$	bneck, 3x3	72	24	-	RE	1
$56^2 \times 24$	bneck, 5x5	72	40	✓	RE	2
$28^2 \times 40$	bneck, 5x5	120	40	✓	RE	1
$28^2 \times 40$	bneck, 5x5	120	40	✓	RE	1
$28^2 \times 40$	bneck, 3x3	240	80	-	HS	2
$14^2 \times 80$	bneck, 3x3	200	80	-	HS	1
$14^2 \times 80$	bneck, 3x3	184	80	-	HS	1
$14^2 \times 80$	bneck, 3x3	184	80	-	HS	1
$14^2 \times 80$	bneck, 3x3	480	112	✓	HS	1
$14^2 \times 112$	bneck, 3x3	672	112	✓	HS	1
$14^2 \times 112$	bneck, 5x5	672	160	✓	HS	2
$7^2 \times 160$	bneck, 5x5	960	160	✓	HS	1
$7^2 \times 160$	bneck, 5x5	960	160	✓	HS	1
$7^2 \times 160$	conv2d, 1x1	-	960	-	HS	1
$7^2 \times 960$	pool, 7x7	-	-	-	-	1
$1^2 \times 960$	conv2d 1x1, NBN	-	1280	-	HS	1
$1^2 \times 1280$	conv2d 1x1, NBN	-	k	-	-	1

Input	Operator	exp size	#out	SE	NL	s
$224^2 \times 3$	conv2d, 3x3	-	16	-	HS	2
$112^2 \times 16$	bneck, 3x3	16	16	✓	RE	2
$56^2 \times 16$	bneck, 3x3	72	24	-	RE	2
$28^2 \times 24$	bneck, 3x3	88	24	-	RE	1
$28^2 \times 24$	bneck, 5x5	96	40	✓	HS	2
$14^2 \times 40$	bneck, 5x5	240	40	✓	HS	1
$14^2 \times 40$	bneck, 5x5	240	40	✓	HS	1
$14^2 \times 40$	bneck, 5x5	120	48	✓	HS	1
$14^2 \times 48$	bneck, 5x5	144	48	✓	HS	1
$14^2 \times 48$	bneck, 5x5	288	96	✓	HS	2
$7^2 \times 96$	bneck, 5x5	576	96	✓	HS	1
$7^2 \times 96$	bneck, 5x5	576	96	✓	HS	1
$7^2 \times 96$	conv2d, 1x1	-	576	✓	HS	1
$7^2 \times 576$	pool, 7x7	-	-	-	-	1
$1^2 \times 576$	conv2d 1x1, NBN	-	1024	-	HS	1
$1^2 \times 1024$	conv2d 1x1, NBN	-	k	-	-	1

The best and most efficient architectures today are found automatically

Source: MobileNetV3 (2019)

Motivation - Summary

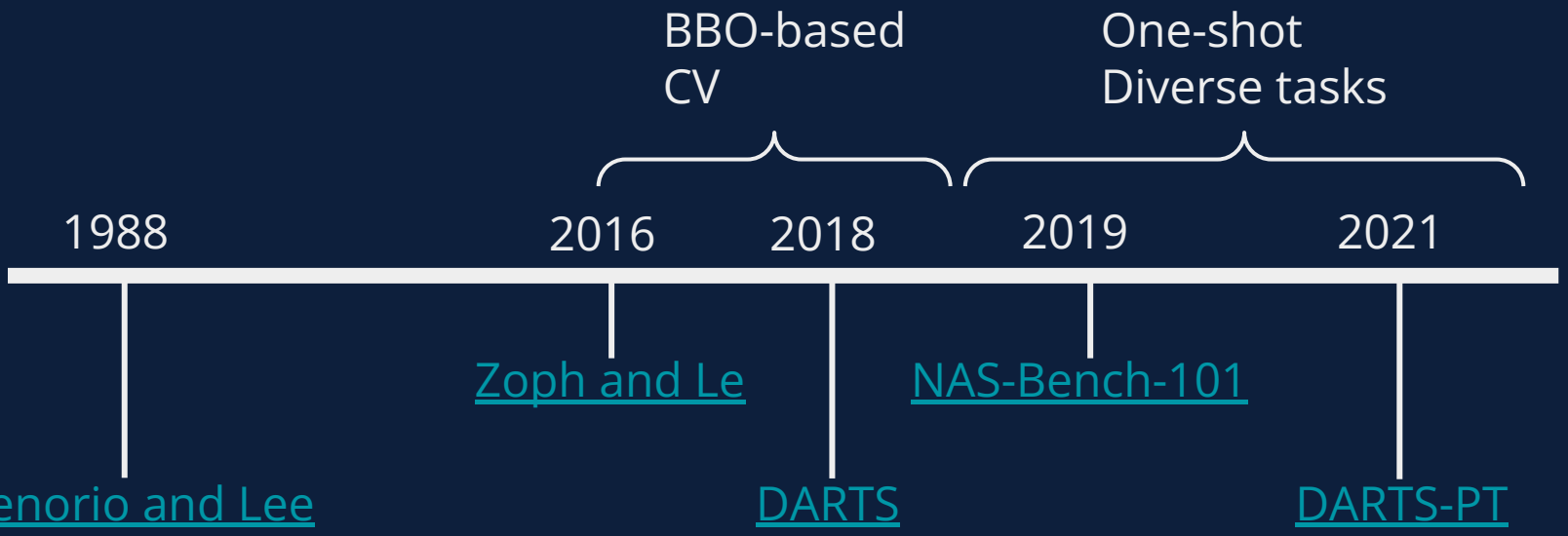
- Widely-used benchmarks
- New datasets
- Constrained / multi-objective problems

- Democratizing deep learning
  - Latest techniques are just a few GPU-hours

NAS: A History

Studied since at least the late 1980s

Resurgence in late 2016



NAS: Basic Definition

- Define a search space ***A,***

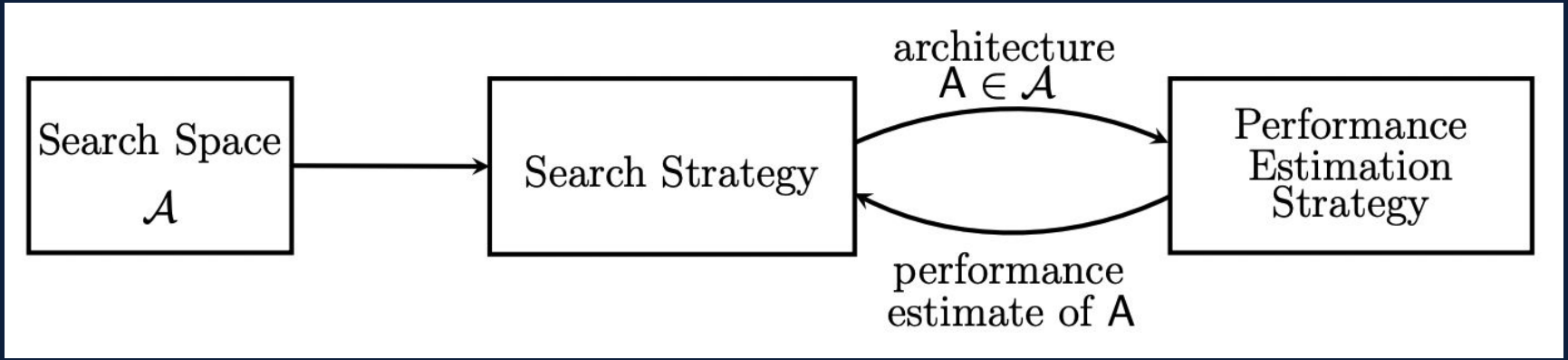
$$\min_{a \in \mathcal{A}} \quad \mathcal{L}_{\text{val}}\left(w^*(a), a\right)$$

$$\text{s.t.} \quad w^*(a) = \text{argmin}_w \quad \mathcal{L}_{\text{train}}\left(w, a\right)$$

Three Pillars of NAS

- Search space
- Search strategy
- Performance estimation strategy

} Coupled, for one-shot methods

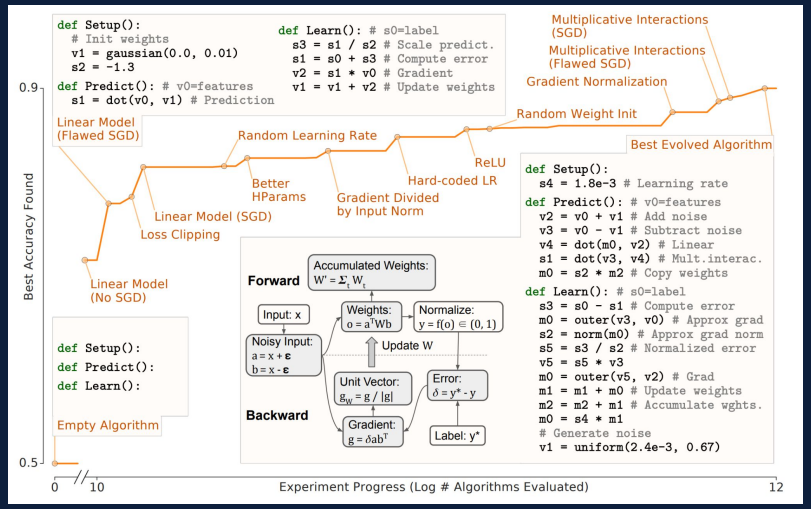


Elsken et al. (2018)

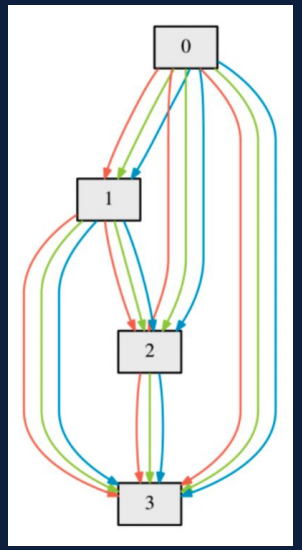
Roadmap - Part 1

- Motivation and introduction
- Search spaces
  - Macro
  - Cell-based
  - Hierarchical
  - Encodings
- Black-box optimization methods
  - Baselines
  - Bayesian optimization
  - Evolution
- Performance prediction

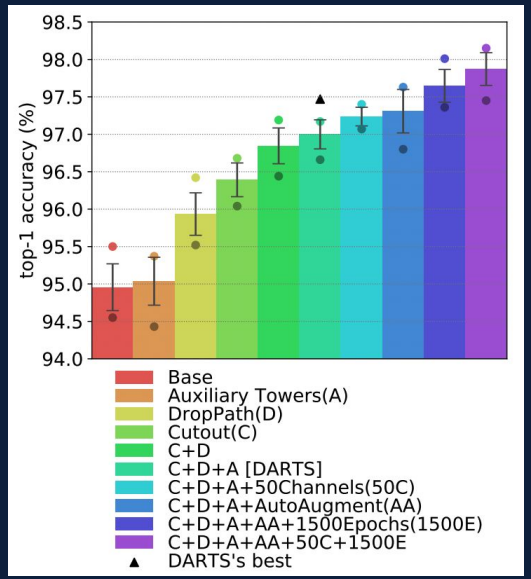
Search Spaces: Exploration vs. Exploitation



[AutoML-Zero (2020)]



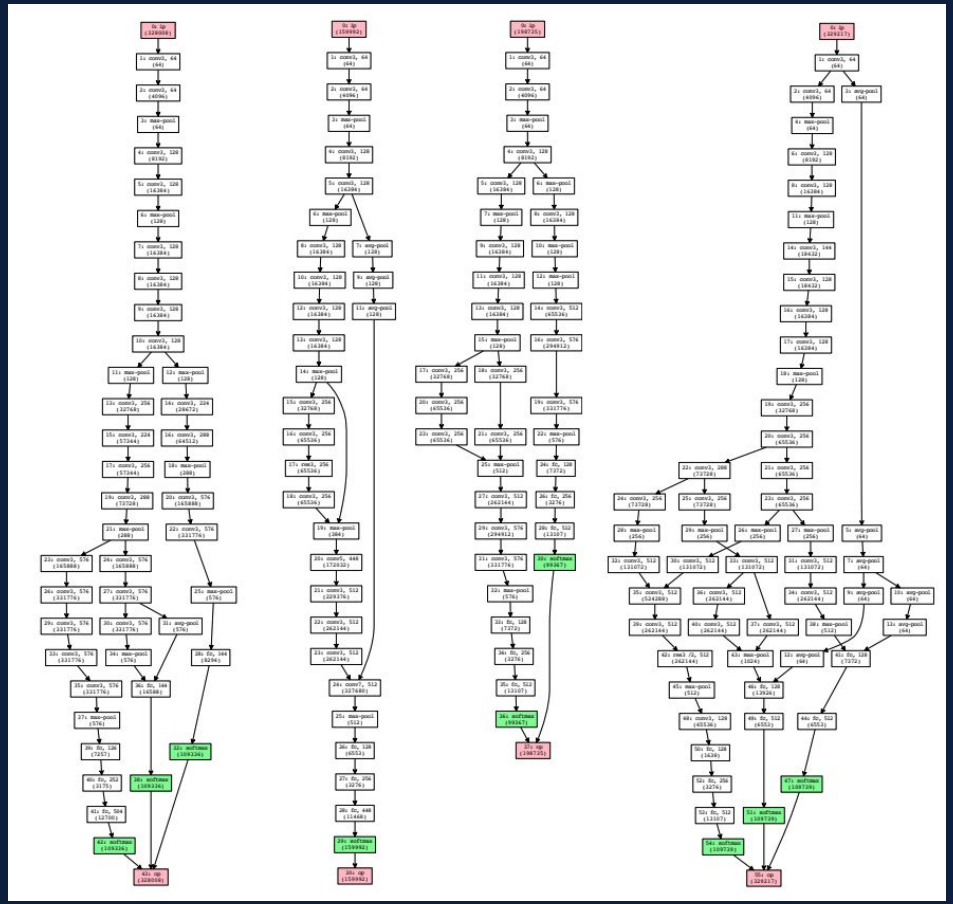
[DARTS (2018)]



[Yang et al. (2019)]

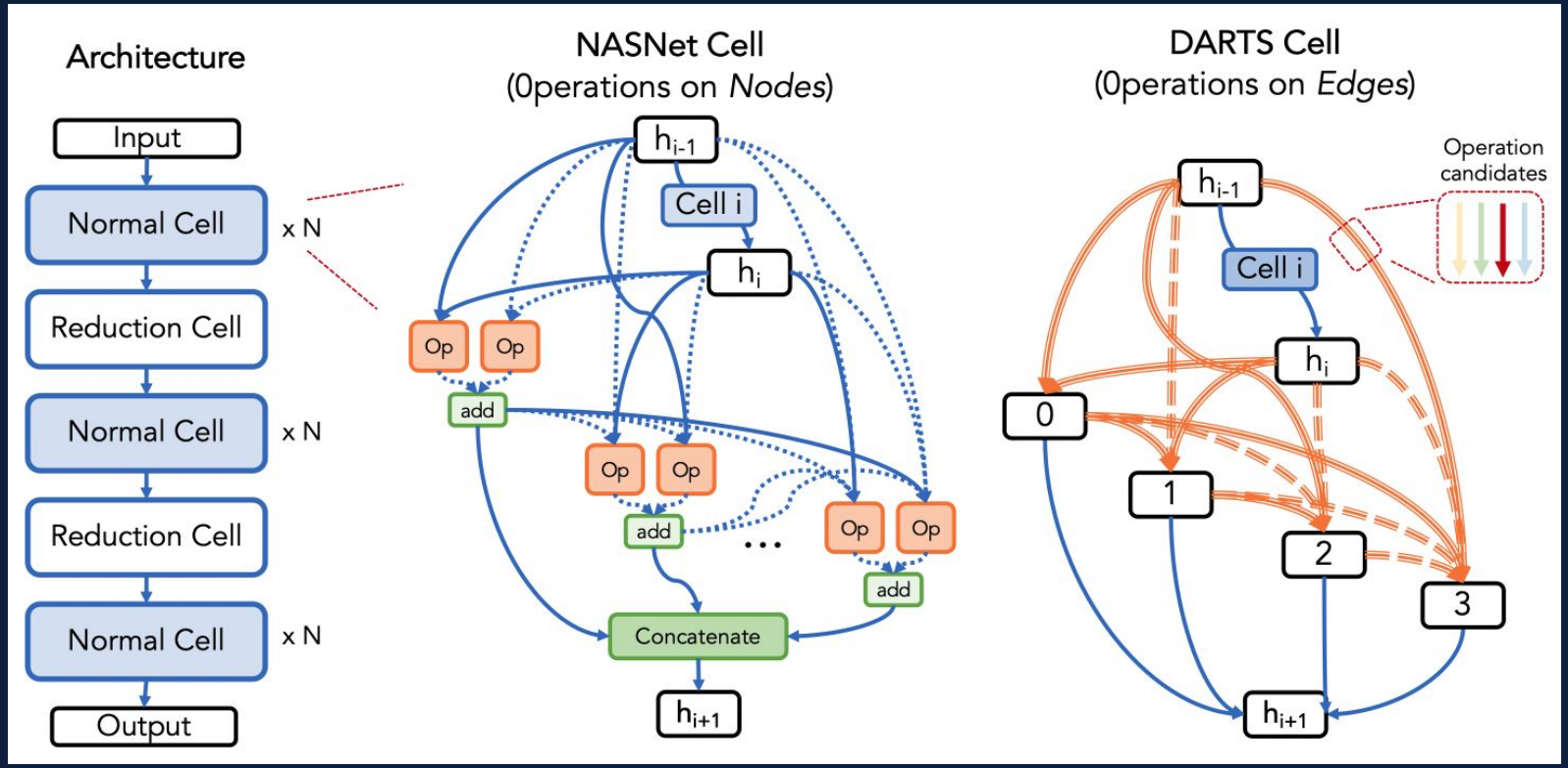
Macro Search Spaces

- Define a set of operations
- Iteratively add more nodes



(NASBOT 2018)

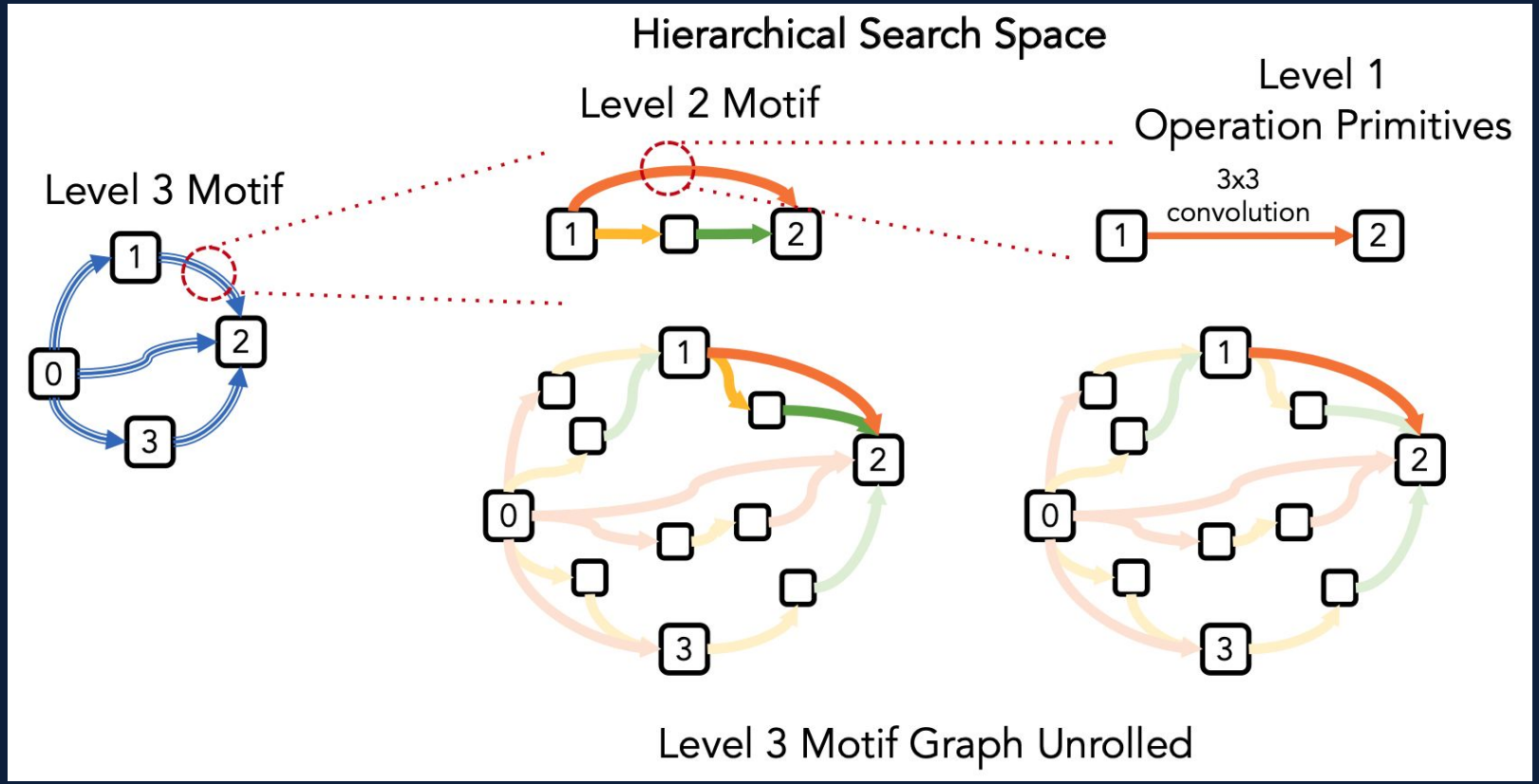
Cell-based search spaces



NASNet (2017)

DARTS (2018)

Hierarchical Search Spaces

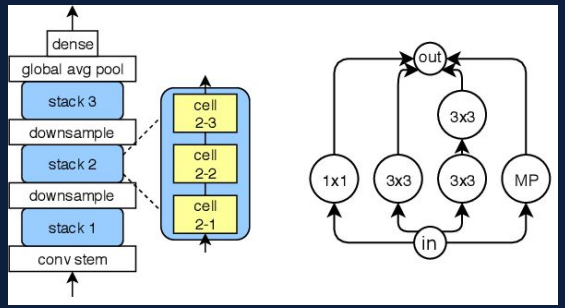


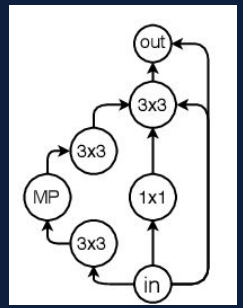
Liu et al. (2017)

Ru et al. (2020)

NAS-Bench-101

- Size 423k
- Used to **simulate** NAS experiments
- Allows for more principled research
  - Fixed training pipeline
  - Can run many trials






```python
# Load the data from file (this will take some time)
nasbench = api.NASBench('/path/to/nasbench.tfrecord')

# Create an Inception-like module (5x5 convolution replaced with two 3x3
# convolutions).
model_spec = api.ModelSpec(
    # Adjacency matrix of the module
    matrix=[[0, 1, 1, 1, 0, 1, 0],    # input layer
            [0, 0, 0, 0, 0, 0, 1],    # 1x1 conv
            [0, 0, 0, 0, 0, 0, 1],    # 3x3 conv
            [0, 0, 0, 0, 0, 1, 0],    # 5x5 conv (replaced by two 3x3's)
            [0, 0, 0, 0, 0, 0, 1],    # 5x5 conv (replaced by two 3x3's)
            [0, 0, 0, 0, 0, 0, 1],    # 3x3 max-pool
            [0, 0, 0, 0, 0, 0, 0]],   # output layer
    # Operations at the vertices of the module, matches order of matrix
    ops=[INPUT, CONV1X1, CONV3X3, CONV3X3, CONV3X3, MAXPOOL3X3, OUTPUT])

# Query this model from dataset, returns a dictionary containing the metrics
# associated with this model.
data = nasbench.query(model_spec)
```

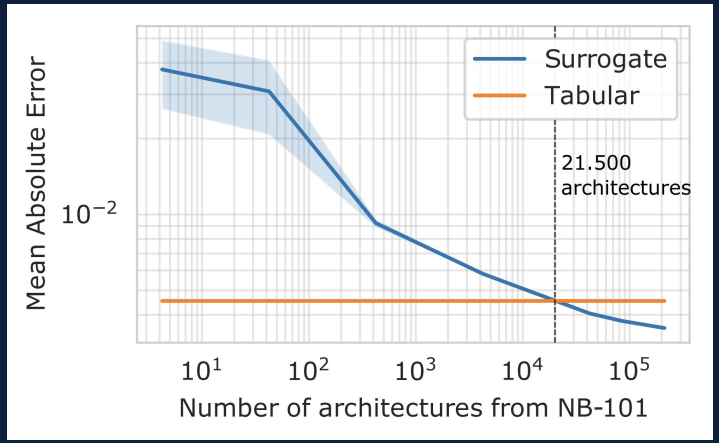
[NAS-Bench-101 (2019)]

NAS Benchmarks

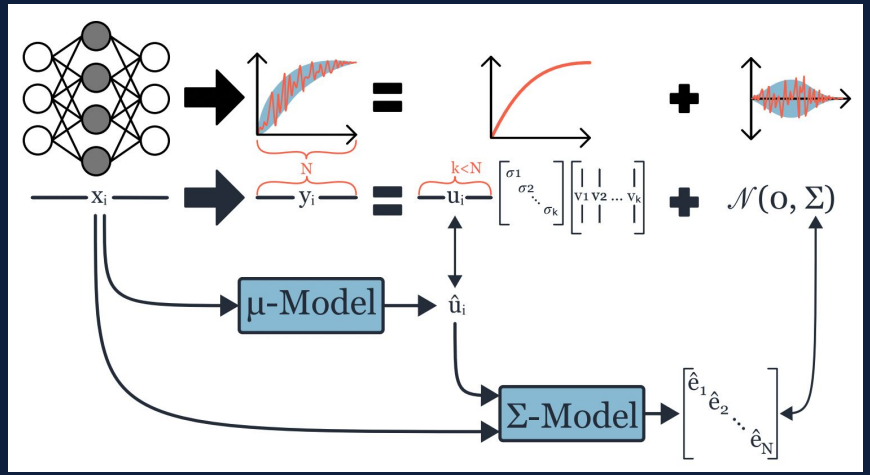
		Queryable						
Benchmark	**Size**	**Tab.**	**Surr.**	**LCs**	**Macro**	**One-Shot**	**Task**	**#Tasks**
NAS-Bench-101	423k	✓				✗	Image class.	1
NATS-Bench-TSS (NAS-Bench-201)	6k	✓		✓		✓	Image class.	3
NATS-Bench-SSS	32k	✓		✓	✓	✓	Image class.	3
NAS-Bench-NLP	$> 10^{53}$			✓		✗	NLP	1
NAS-Bench-1Shot1	364k	✓				✓	Image class.	1
Surr-NAS-Bench-DARTS (NAS-Bench-301)	10^{18}		✓			✓	Image class.	1
Surr-NAS-Bench-FBNet	10^{21}		✓			✗	Image class.	1
NAS-Bench-ASR	8k	✓			✓	✓	ASR	1
TransNAS-Bench-101-Micro	4k	✓		✓		✓	Var. CV	7
TransNAS-Bench-101-Macro	3k	✓		✓	✓	✗	Var. CV	7
NAS-Bench-111	423k		✓	✓		✗	Image class.	1
NAS-Bench-311	10^{18}		✓	✓		✓	Image class.	1
NAS-Bench-NLP11	$> 10^{53}$		✓	✓		✗	NLP	1
NAS-Bench-MR	10^{23}		✓		✓	✗	Var. CV	9
NAS-Bench-360	Var.				✓	✓	Var.	30
NAS-Bench-Macro	6k	✓			✓	✗	Image class.	1
HW-NAS-Bench-201	6k	✓		✓		✓	Image class.	3
HW-NAS-Bench-FBNet	10^{21}					✗	Image class.	1

Surrogate NAS Benchmarks

- Surr-NAS-Bench-DARTS (NAS-Bench-301)
- Surr-NAS-Bench-FBNet
- NAS-Bench-111
- NAS-Bench-311
- NAS-Bench-NLP11



Surr-NAS-Bench (2020)

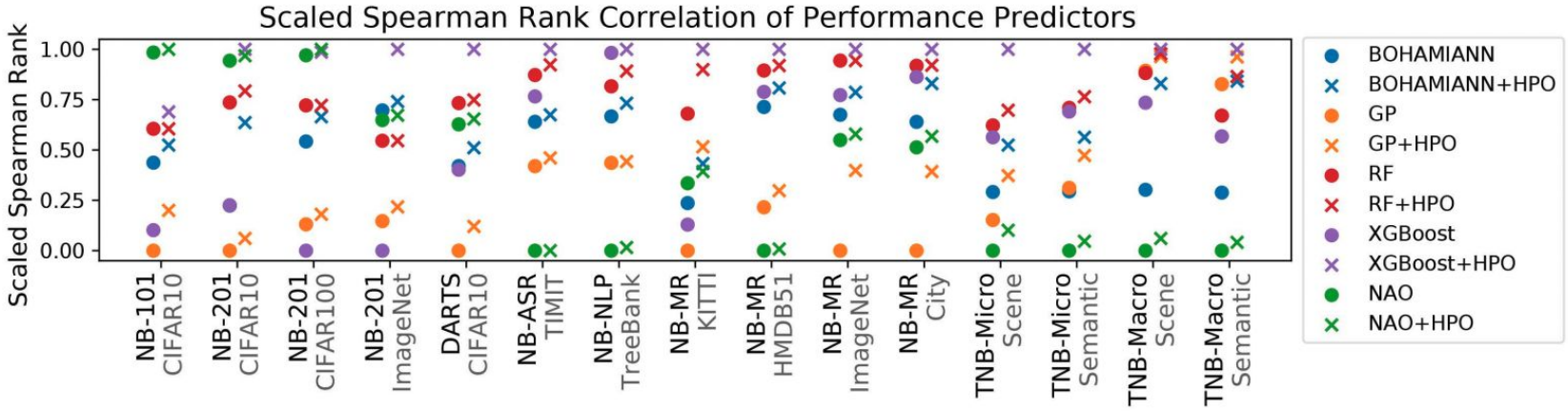


NAS-Bench-x11 (2021)

NAS-Bench-Suite (25 tasks)

	NAS Algorithms					Performance Predictors				
	RS	RE	BANANAS	LS	NPENAS	GP	BOHAM.	RF	XGB	NAO
Avg.Rank, 101&201	4.50	3.00	3.50	**1.50**	2.50	4.67	2.83	2.17	4.17	**1.17**
Avg. Rank, non-101&201	3.06	**2.11**	2.83	3.13	3.87	4.08	3.06	**1.33**	2.46	4.08

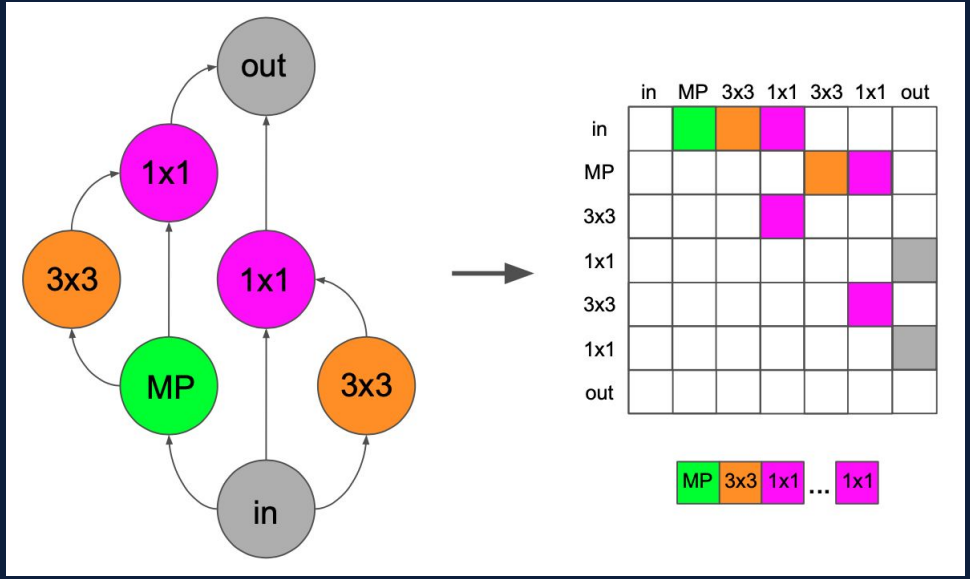
- Conclusions drawn from just the popular NAS-Bench-101 and NAS-Bench-201 can be misleading!



NAS-Bench-Suite (2022) https://github.com/automl/naslib

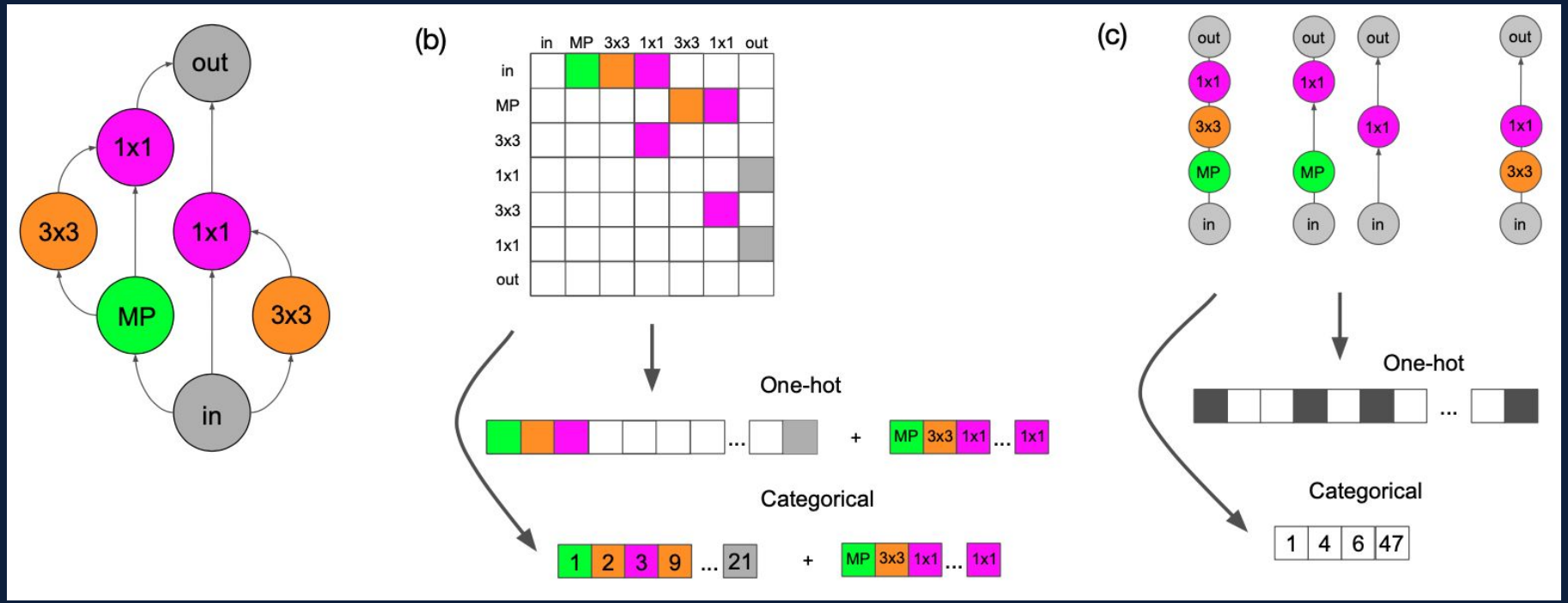
Encodings for NAS

Most NAS algorithms search over DAG-based architectures, which must be encoded into a tensor



White et al. (2020)

Encodings for NAS



NAS encoding-dependent subroutines

Many NAS algos can be composed from three subroutines

- Sample random architecture
- Perturb architecture
- Train predictor model

Algorithm 1 BANANAS

Input: Search space A, dataset D, parameters t_0, T, M, c, x, acquisition function ϕ, function $f(a)$ returning validation error of a after training.

1. Draw t_0 architectures $a_0, \ldots, a_{t_0}$ uniformly at random from A and train them on D.
2. For t from t_0 to T,
   i. Train an ensemble of neural predictors on $\{(a_0, f(a_0)), \ldots, (a_t, f(a_t))\}$ using the path encoding to represent each architecture.
   ii. Generate a set of c candidate architectures from A by randomly mutating the x architectures a from $\{a_0, \ldots, a_t\}$ that have the lowest value of $f(a)$.
   iii. For each candidate architecture a, evaluate the acquisition function $\phi(a)$.
   iv. Denote a_{t+1} as the candidate architecture with minimum $\phi(a)$, and evaluate $f(a_{t+1})$.

Output: $a^* = \text{argmin}_{t=0,\ldots,T} f(a_t)$.

Algorithm 1 Aging Evolution

```
population ← empty queue                          ▷ The population.
history ← ∅                                       ▷ Will contain all models.
while |population| < P do                         ▷ Initialize population.
    model.arch ← RANDOMARCHITECTURE()
    model.accuracy ← TRAINANDEVAL(model.arch)
    add model to right of population
    add model to history
end while
while |history| < C do                            ▷ Evolve for C cycles.
    sample ← ∅                                    ▷ Parent candidates.
    while |sample| < S do
        candidate ← random element from population
                                                  ▷ The element stays in the population.
        add candidate to sample
    end while
    parent ← highest-accuracy model in sample
    child.arch ← MUTATE(parent.arch)
    child.accuracy ← TRAINANDEVAL(child.arch)
    add child to right of population
    add child to history
    remove dead from left of population           ▷ Oldest.
    discard dead
end while
return highest-accuracy model in history
```

Algorithm 1 Bayesian Optimized Neural Architecture Search (BONAS). $\mathcal{A}$ is the given search space, N is the number of initial architectures, k is the ratio of GCN / BLR update times.

1: initialize random N fully-trained architectures: $\mathcal{D} = \{(A_i, X_i, t_i)\}_{i=1}^{N}$ from search space $\mathcal{A}$;
2: initial training of GCN using $\mathcal{D}$ with proposed loss;
3: replace the final layer of GCN with BLR;
4: initialize Sampler;
5: **repeat**
6: **for** iteration$= 1, 2, \ldots, k$ **do**
7: sample candidate pool $\mathcal{C}$ from $\mathcal{A}$;
8: **for** each candidate m in $\mathcal{C}$ **do**
9: embed m using GCN;
10: compute μ and σ^2 in (4) and (5) using BLR;
11: compute expected improvement (EI) in (2);
12: **end for**
13: $M \leftarrow$ candidate with the highest EI score;
14: fully train M to obtain its actual performance;
15: add M and its actual performance to $\mathcal{D}$;
16: update BLR using the enlarged $\mathcal{D}$;
17: update Sampler;
18: **end for**
19: retrain GCN using the enlarged $\mathcal{D}$ with proposed loss;
20: **until** stop criterion satisfy.

White et al. (2020)

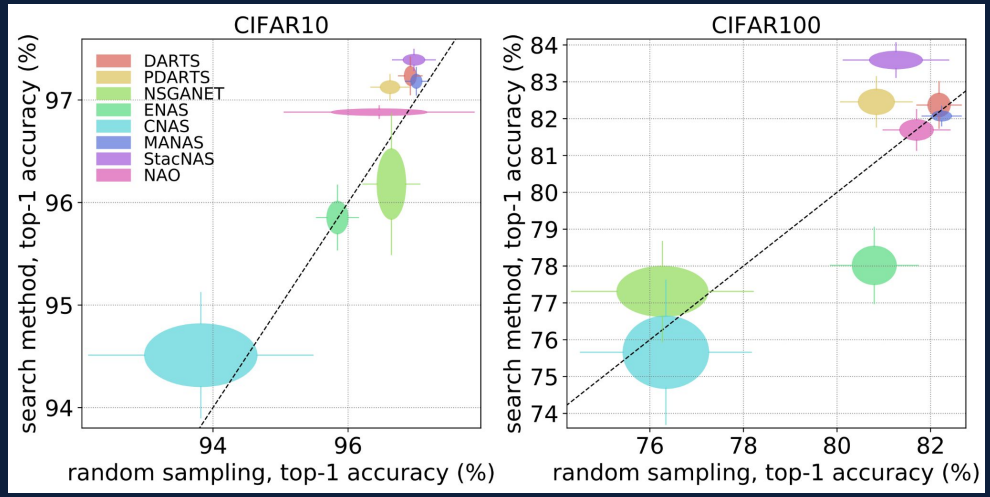
Roadmap - Part 1

- Motivation and introduction
- Search spaces
  - Macro
  - Cell-based
  - Hierarchical
  - Encodings
- Black-box optimization methods
  - Baselines
  - Bayesian optimization
  - Evolution
- Performance prediction

Random Search & Random Sampling

Random search is surprisingly competitive [Li and Talwalkar, 2019], [Yang et al., 2019], [Sciuto et al., 2020]

Random sampling: performance of a randomly drawn architecture.



Yang et al. (2019)

Local Search

- Five lines of code
- Performs surprisingly well on popular benchmarks

Algorithm 1 Local search

Input: Search space A, objective function ℓ, neighborhood function N

1. Pick an architecture $v_1 \in A$ uniformly at random
2. Evaluate $\ell(v_1)$; denote a dummy variable $\ell(v_0) = \infty$; set $i = 1$
3. While $\ell(v_i) < \ell(v_{i-1})$:
   i. Evaluate $\ell(u)$ for all $u \in N(v_i)$
   ii. Set $v_{i+1} = \text{argmin}_{u \in N(v_i)} \ell(u)$; set $i = i + 1$

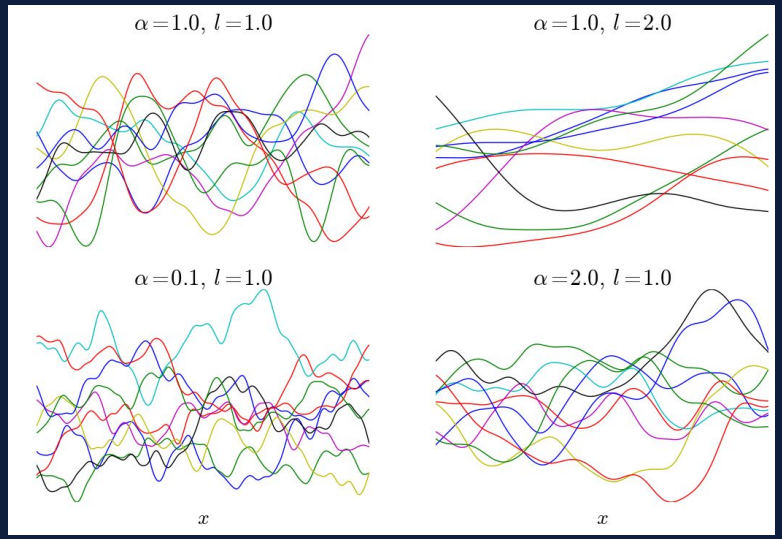
Output: Architecture v_i

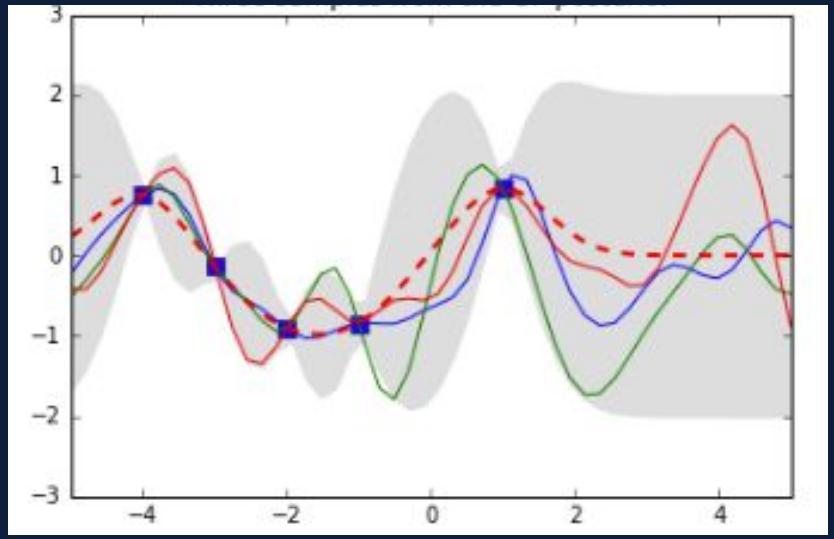
[Ottellander et al. 2020]

[White et al. 2020]

Bayesian optimization

- [NASBOT, 2018], [Auto-Keras, 2018], [NASBOWL, 2020]





Source: http://keyonvafa.com/gp-tutorial/, https://katbailey.github.io/post/gaussian-processes-for-dummies/

“BO + Neural Predictor” Framework

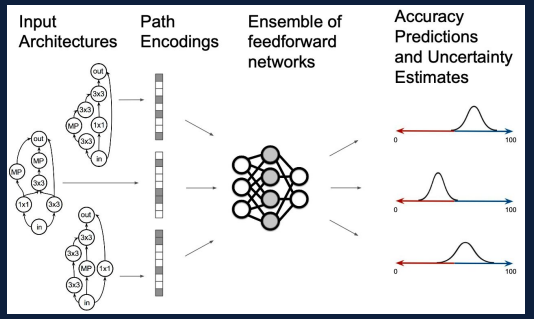
[NASGBO, 2019], [BONAS, 2019], [BANANAS, 2021]

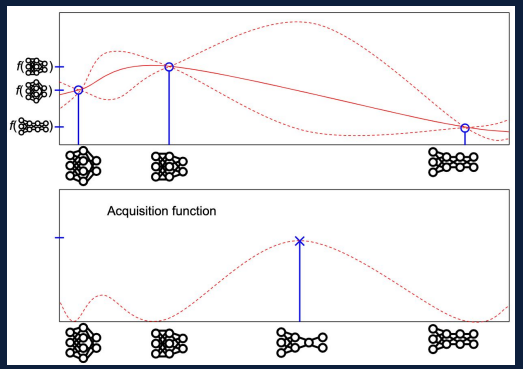
Algorithm 1 BANANAS

Input: Search space A, dataset D, parameters t_0, T, M, c, x, acquisition function ϕ, function $f(a)$ returning validation error of a after training.

1. Draw t_0 architectures $a_0, \ldots, a_{t_0}$ uniformly at random from A and train them on D.
2. For t from t_0 to T,
   - i. Train an ensemble of meta neural networks on $\{(a_0, f(a_0)), \ldots, (a_t, f(a_t))\}$.
   - ii. Generate a set of c candidate architectures from A by randomly mutating the x architectures a from $\{a_0, \ldots, a_t\}$ that have the lowest value of $f(a)$.
   - iii. For each candidate architecture a, evaluate the acquisition function $\phi(a)$.
   - iv. Denote a_{t+1} as the candidate architecture with minimum $\phi(a)$, and evaluate $f(a_{t+1})$.

Output: $a^* = \text{argmin}_{t=0,\ldots,T} f(a_t)$.





Train 10 arch.’s each iteration

“BO + Neural Predictor” Components

Algorithm 1 BANANAS

Input: Search space A, dataset D, parameters t_0, T, M, c, x, acquisition function ϕ, function $f(a)$ returning validation error of a after training.

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Output: $a^* = \text{argmin}_{t=0,\ldots,T} f(a_t)$.

- Architecture encoding
- Uncertainty calibration
- Neural predictor architecture
- Acquisition function
- Acquisition optimization strategy

BANANAS

[BANANAS, 2021]

Algorithm 1 BANANAS

Input: Search space A, dataset D, parameters t_0, T, M, c, x, acquisition function ϕ, function $f(a)$ returning validation error of a after training.

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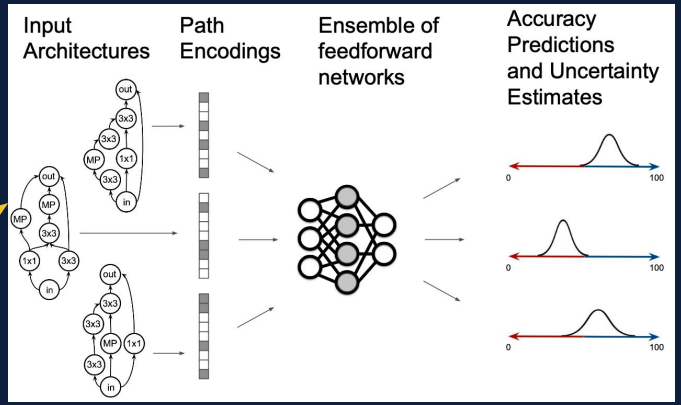


Path encoding, ensemble

Small mutations

Independent Thompson Sampling

Evolution

Algorithm 1 General Evolutionary Algorithm

Input: Initial population of architecture data $\mathcal{D}_0 = (a_i, y_i)_{i=1}^{N_0}$, objective function f, total number of evolution steps T

Output: The optimal architecture a_T^*

for $t = 1, \ldots, T$ **do**

Sample a set of parent architectures $\mathcal{S}_{parents} = \{(a_j, y_j)\}_{j=1}^{N_p}$ from the population $\mathcal{D}_{t-1}$

Generate children architectures by mutating parent architectures and evaluate their performance to obtain $\mathcal{S}_{children} = \{(a_k, y_k)\}_{k=1}^{N_c}$

Update the population with $\mathcal{S}_{children}$ to obtain $\mathcal{D}_t$

end for

Decisions: sampling the initial population, selecting the parents, generating the offspring

Real et al. (2018)

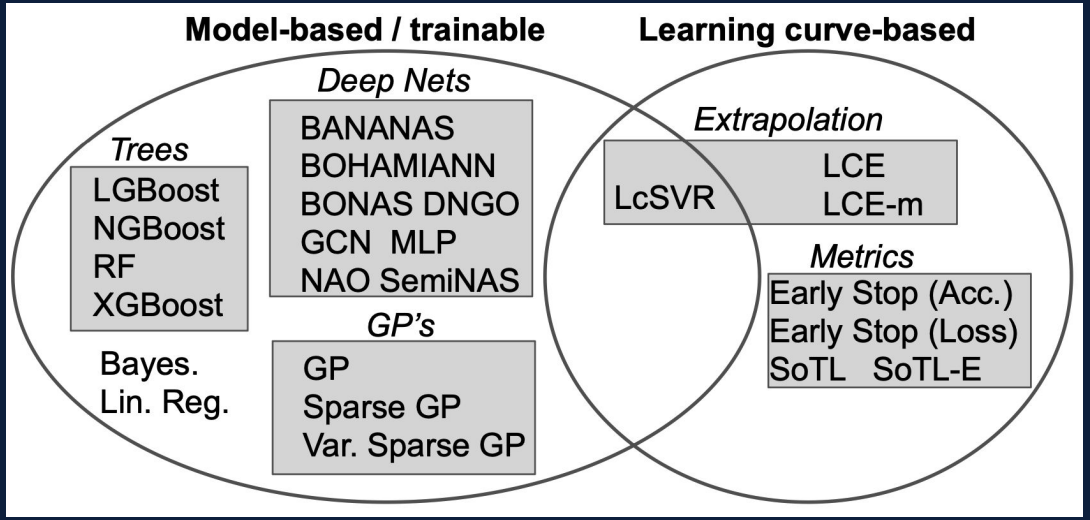
Roadmap - Part 1

- Motivation and introduction
- Search spaces
  - Macro
  - Cell-based
  - Hierarchical
  - Encodings
- Black-box optimization methods
  - Baselines
  - Bayesian optimization
  - Evolution
- Performance prediction

Performance Predictors

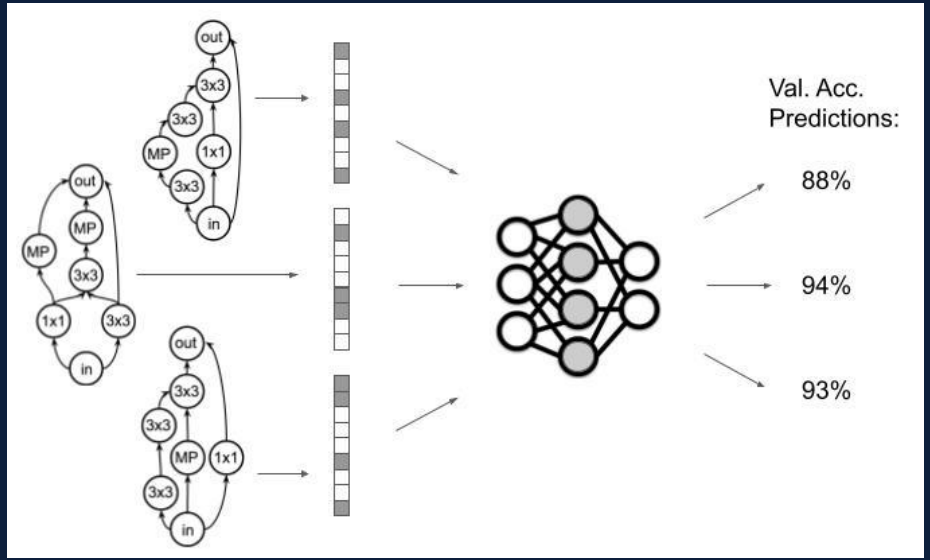
Any technique which predicts the (relative) accuracy of an architecture, without fully training it.

- ***Initialization**:* performs any necessary pre-computation
- ***Query**:* take any architecture as input, and output predicted accuracy



Model-Based Predictors

- Supervised learning - regression
  - X - the architecture encoding (e.g. one-hot adjacency matrix)
  - Y - validation accuracy of trained architecture



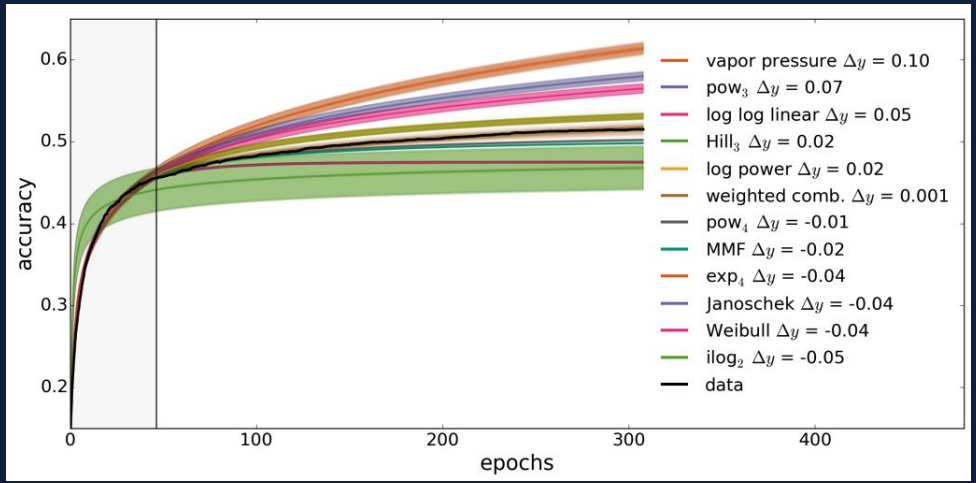
[White et al. 2019]

- Gaussian processes [Kandasamy et al. 2018], [Jin et al. 2018]
- Boosted trees [Luo et al. 2020], [Siems et al. 2020]
- GNNs [Shi et al. 2019], [Wen et al. 2019]
- Specialized encodings [White et al. 2019], [Ning et al. 2020]

High init time, low query time

Learning curve based predictors

- Learning curve extrapolation
  - Fit partial learning curve to parametric model [Domhan et al. 2015]
  - Bayesian NN [Klein et al. 2017]
- Training statistics
  - Early stopping (val acc) [Elsken et al. 2018]
  - Sum of training losses [Ru et al. 2020]



[Elsken et al. 2018]

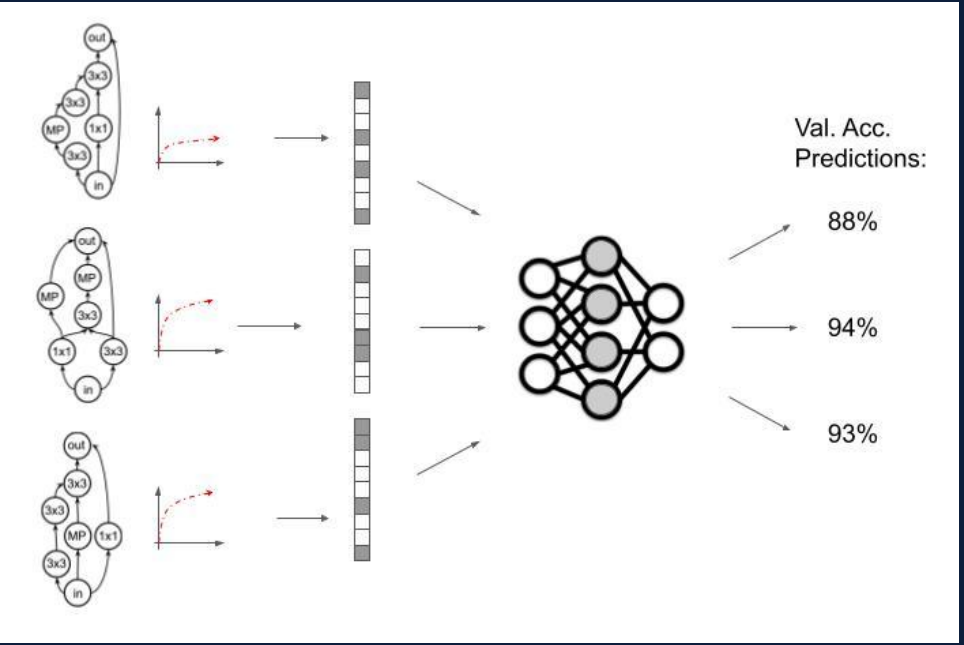
No init time, high query time

Hybrid model-based + LC predictors

Train a model, using partial learning curve + hyperparams, to predict final accuracy

- First and second derivatives as features, SVR [Baker et al. 2017]
- Full LC as features, Bayesian NN [Klein et al. 2017]

High init time, high query time

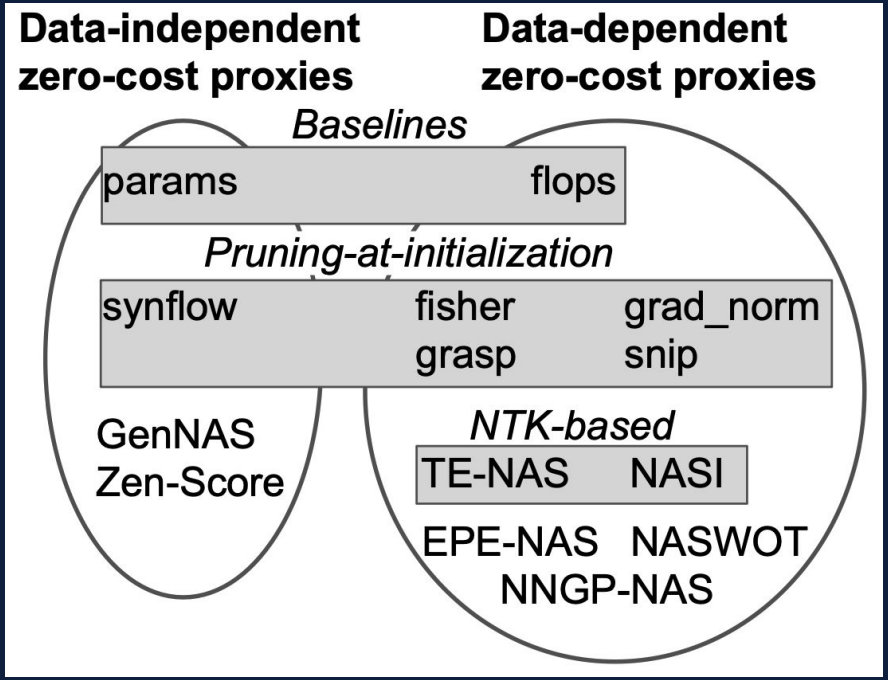


“Zero-cost” proxies

Compute a statistic of an architecture in 3-5 seconds

- Jacobian covariance [Mellor et al. 2020]
- Synaptic Flow [Abdelfattah et al. 2021]
  - SNIP [Lee et al. 2018]

Low init time, low query time



[Abdelfattah et al. 2021]

$$\texttt{snip} : \mathcal{S}_p(\theta) = \left| \frac{\partial \mathcal{L}}{\partial \theta} \odot \theta \right|, \qquad \texttt{grasp} : \mathcal{S}_p(\theta) = -(H \frac{\partial \mathcal{L}}{\partial \theta}) \odot \theta, \qquad \texttt{synflow} : \mathcal{S}_p(\theta) = \frac{\partial \mathcal{L}}{\partial \theta} \odot \theta$$

OMNI: The Omnipotent Predictor

Algorithm 1 OMNI predictor

Input: Search space A, dataset D, initialization time budget B_{init}, query time budget B_{query}.
Initialization():

- $\mathcal{D}_{\text{train}} \leftarrow \emptyset$
- While $t < B_{\text{init}}$
  - Draw an architecture a randomly from A
  - Train a to completion to compute val. accuracy y_a
  - $\mathcal{D}_{\text{train}} \leftarrow \mathcal{D}_{\text{train}} \cup \{(a, y_a)\}$
- Train an NGBoost model m to predict the final val. accuracy of architectures from $\mathcal{D}_{\text{train}}$, using the architecture encoding, SoTL-E, and Jacob. cov. as input features.

Query(architecture a_{test}):

- While $t < B_{\text{query}}$, train a_{test}
- Compute SoTL-E using the partial learning curve, and compute Jacob. cov., and the arch. encoding of a_{test}
- Predict val. acc. of a_{test} using m and the above features.

[White et al. (2021)]

Thanks! Questions?

- Search spaces
  - Macro
  - Cell-based
  - Hierarchical
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- Black-box optimization methods
  - Baselines
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Slides (with hyperlinks): https://crwhite.ml/