Neural Architecture Search: The Next Frontier

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

Machine learning automation

NAS Lib

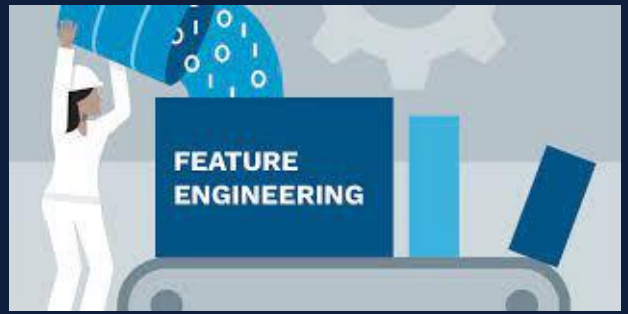
ABACUS.AI

1950s

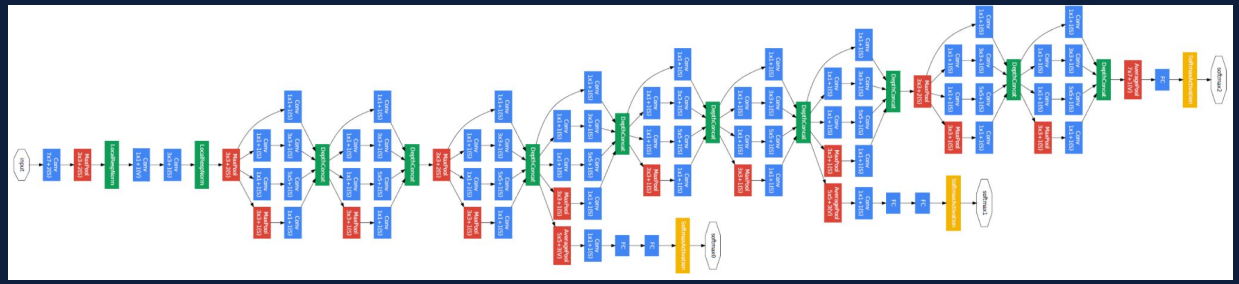
2011

2017

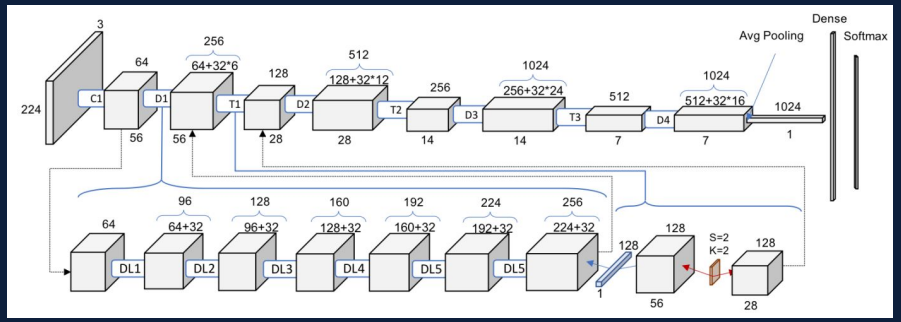
2022



Neural architectures

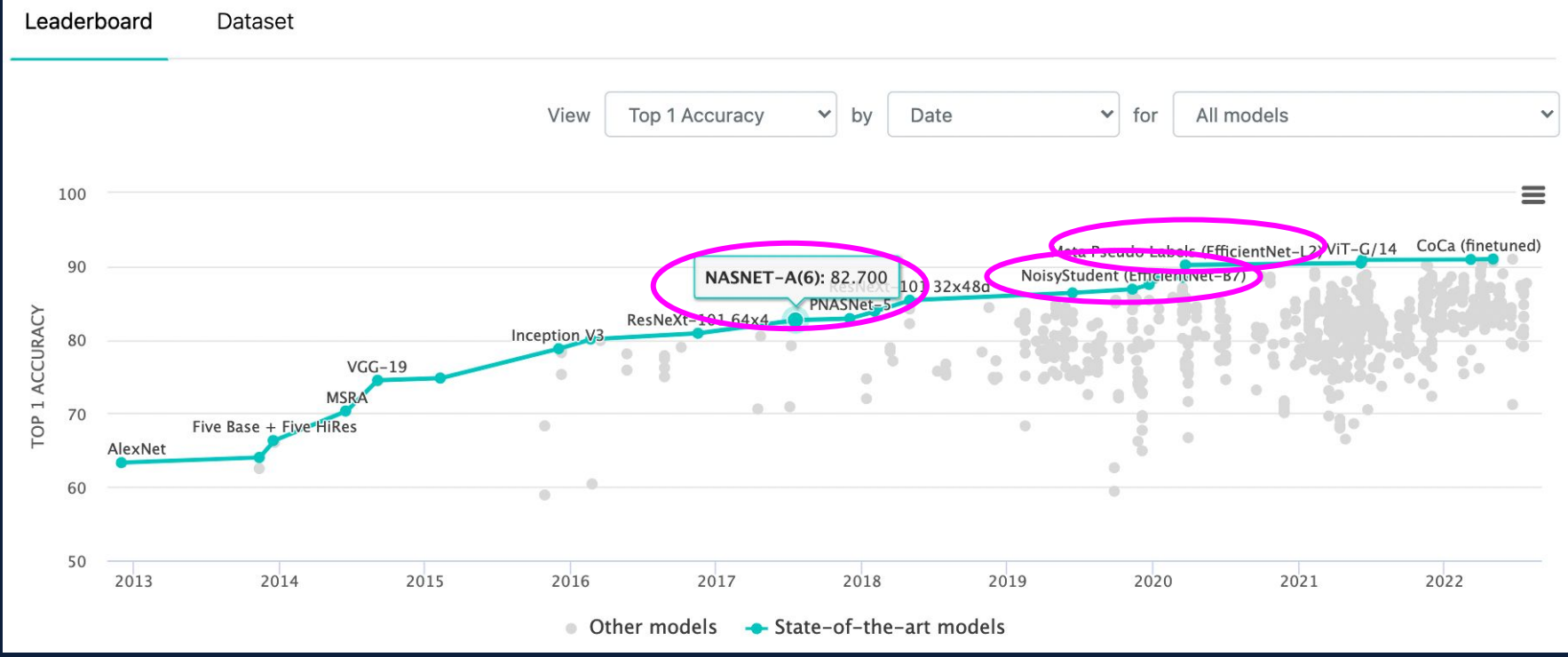


GoogLeNet (2014)



DenseNet (2016)

Image Classification on ImageNet



https://paperswithcode.com/sota/image-classification-on-imagenet

What is NAS?

What is neural architecture search?

Neural architecture search (NAS) is a technique for automatically designing neural networks. NAS algorithms typically use a reinforcement learning (RL) or evolutionary algorithm (EA) to search for an optimal neural network architecture.

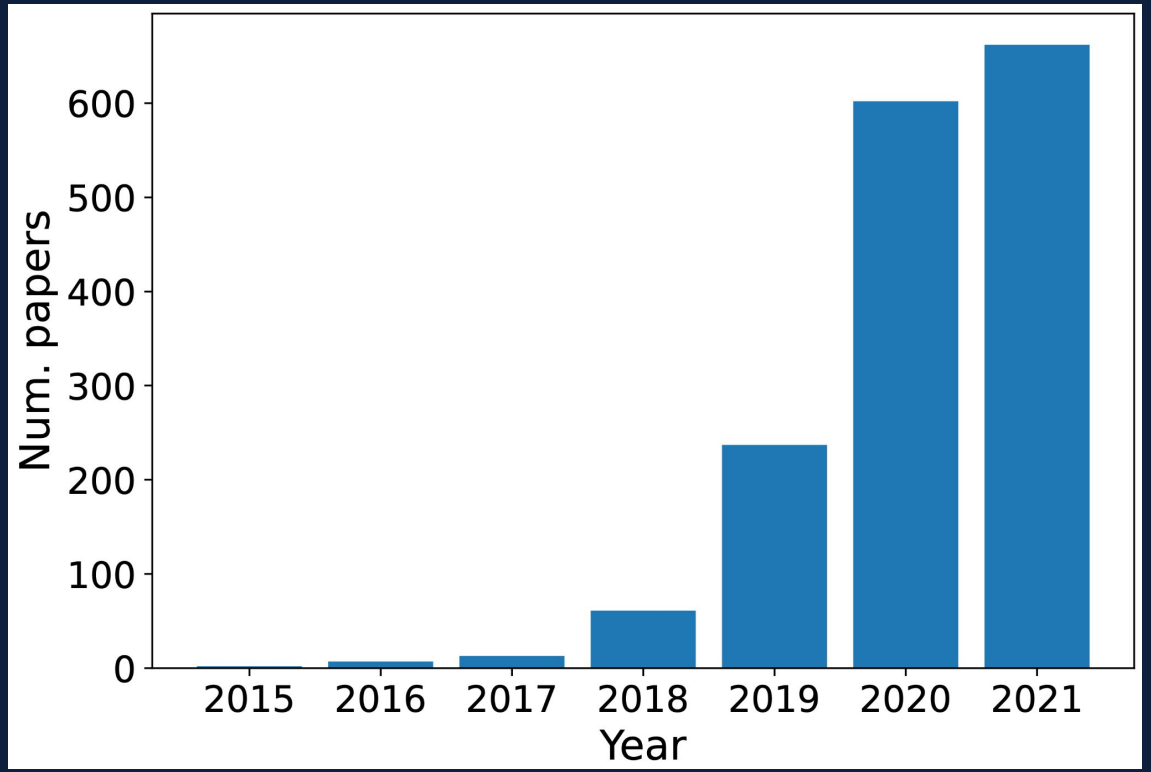
DALL·E My collection

Edit the detailed description

What is neural architecture search? Generate

Neural architecture search

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



Basic Definition

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

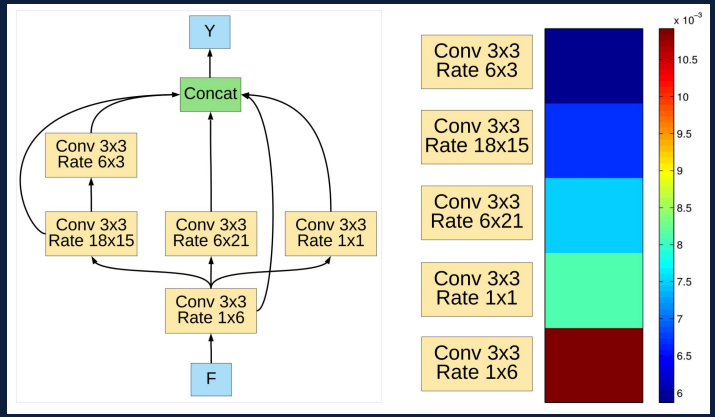
$$\min_{a \in \mathcal{A}} \quad \mathcal{L}_{\text{val}}\left(w^*(a), a\right)$$

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

Diverse datasets / tasks

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	

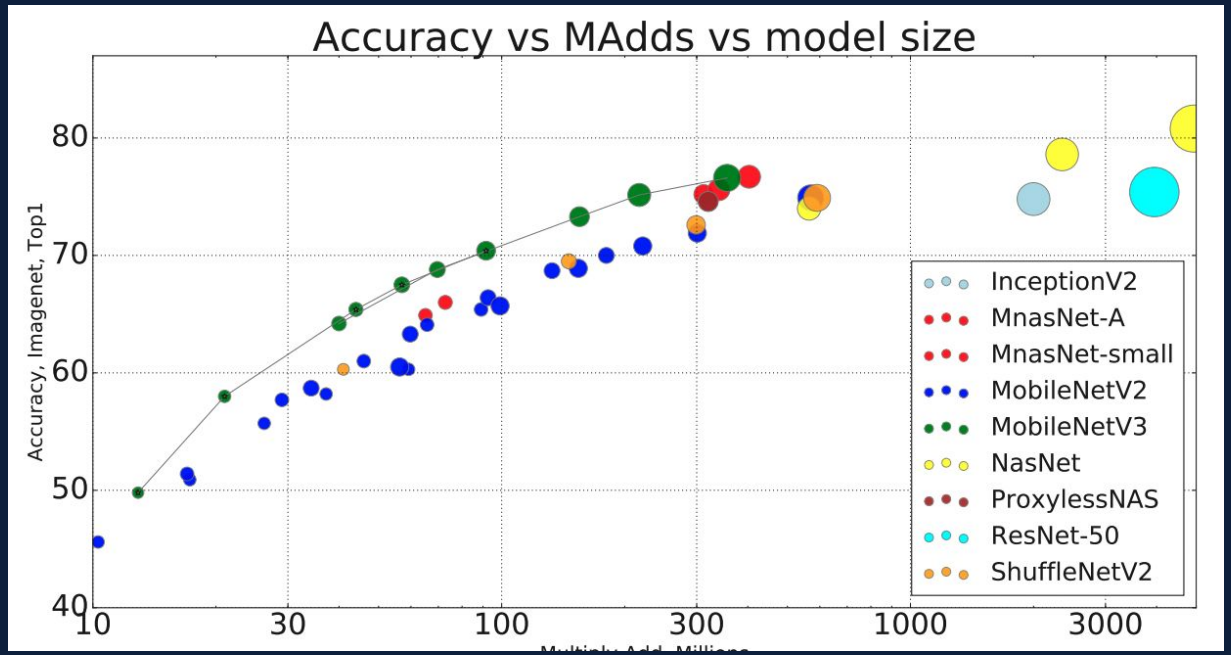
Graph neural networks . . . . .
Generative adversarial network
Dense prediction tasks . . . . .
Adversarial robustness . . . . .
Self-supervised learning for NAS



[NAS-Bench-360 (2021)]

[Chen et al. 2018]

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

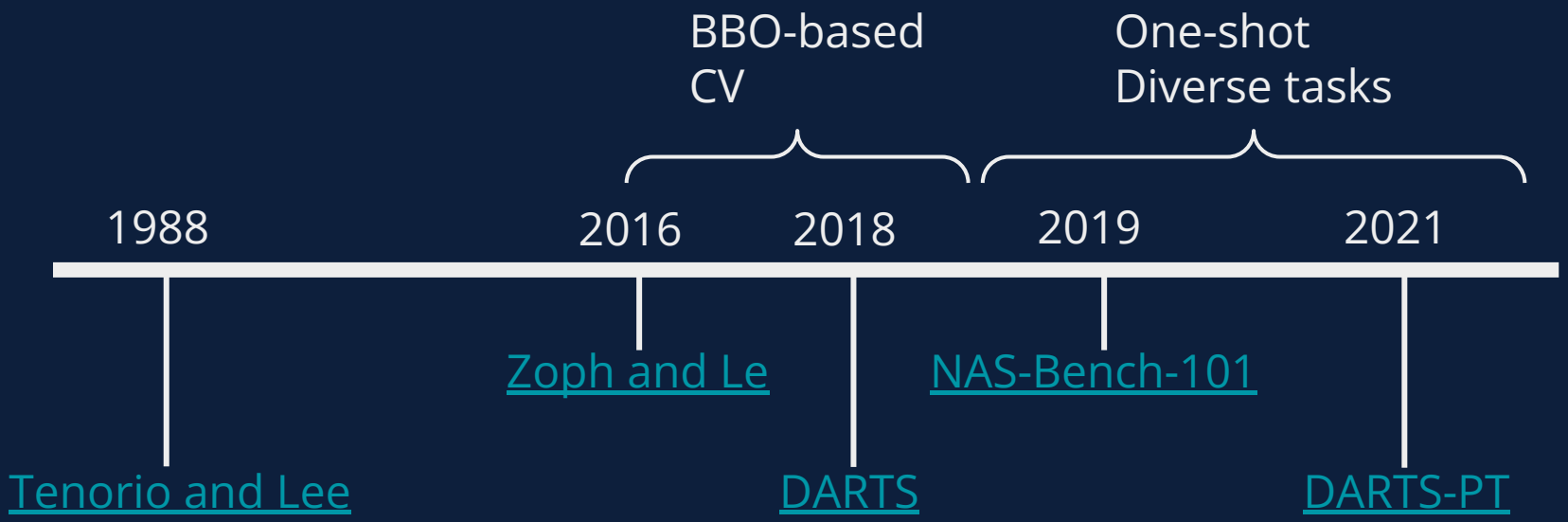
MobileNetV3 (2019)

Motivation - Summary

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

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

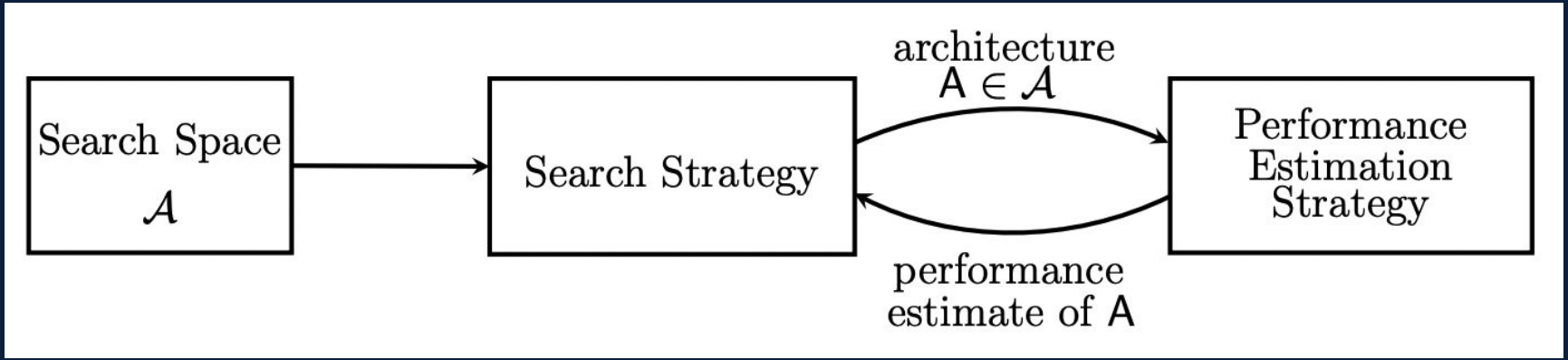
NAS: A History



Three Pillars of NAS

- Search space
- Search strategy
- Performance estimation strategy

} Coupled, for one-shot methods

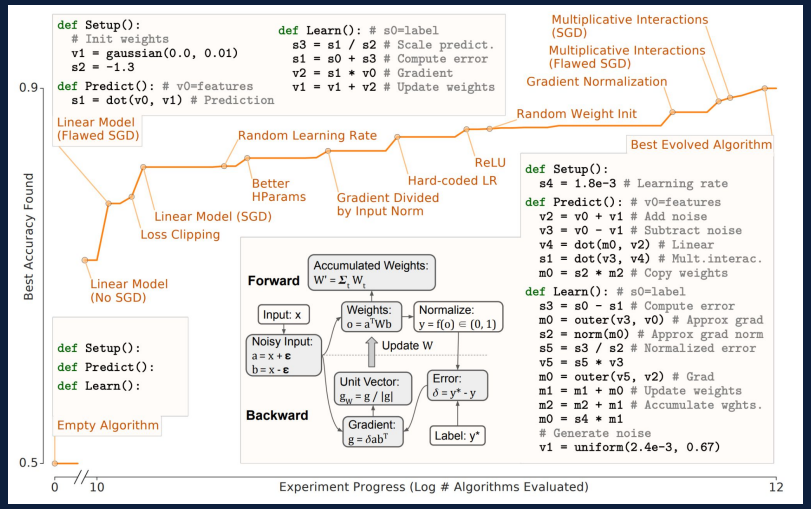


Elsken et al. (2018)

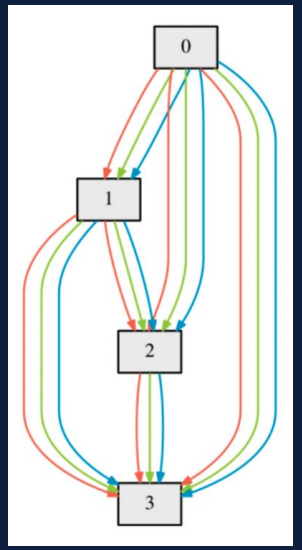
Roadmap

- Introduction
- Search spaces
- Black-box optimization methods
- One-shot methods
- NAS Benchmarks
- Case studies
  - Face Recognition
  - Climate Change
  - Recommender systems

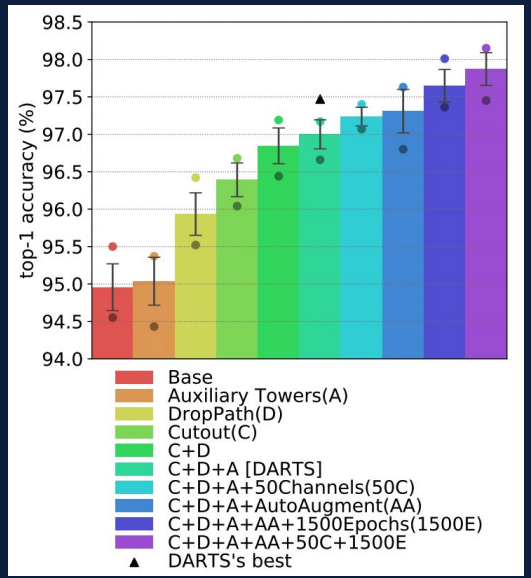
Search Spaces: Exploration vs. Exploitation



[AutoML-Zero (2020)]



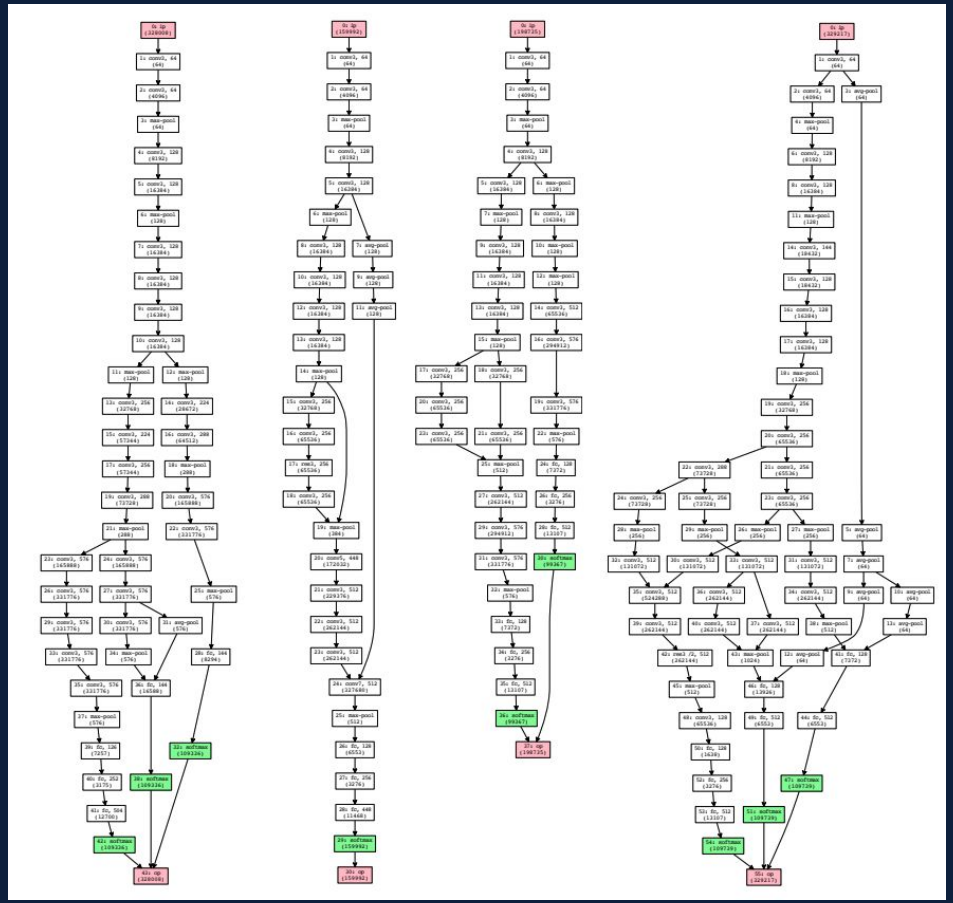
[DARTS (2018)]



[Yang et al. (2019)]

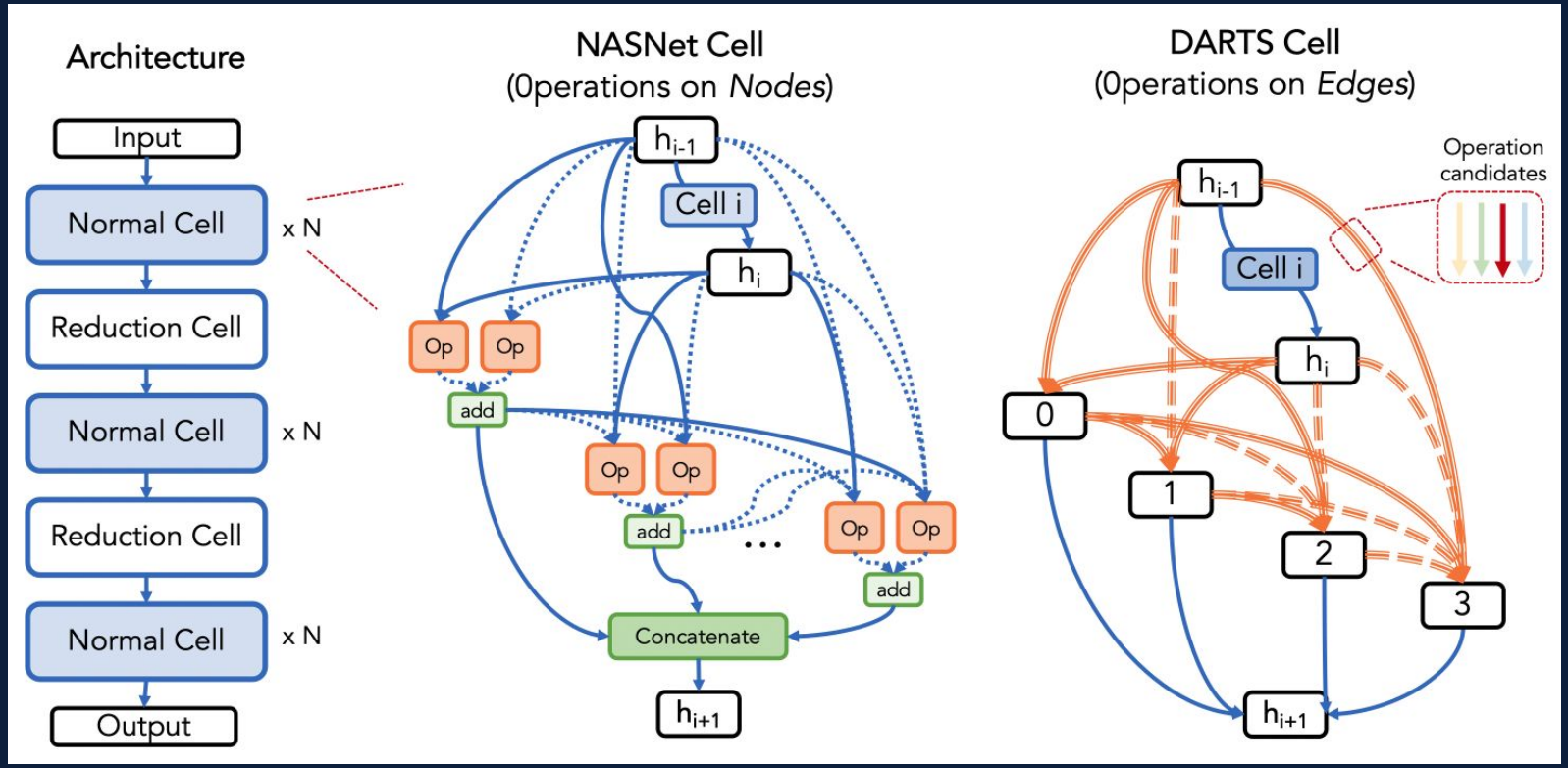
Macro Search Spaces

- Define a set of operations
- Iteratively add more nodes



(NASBOT 2018)

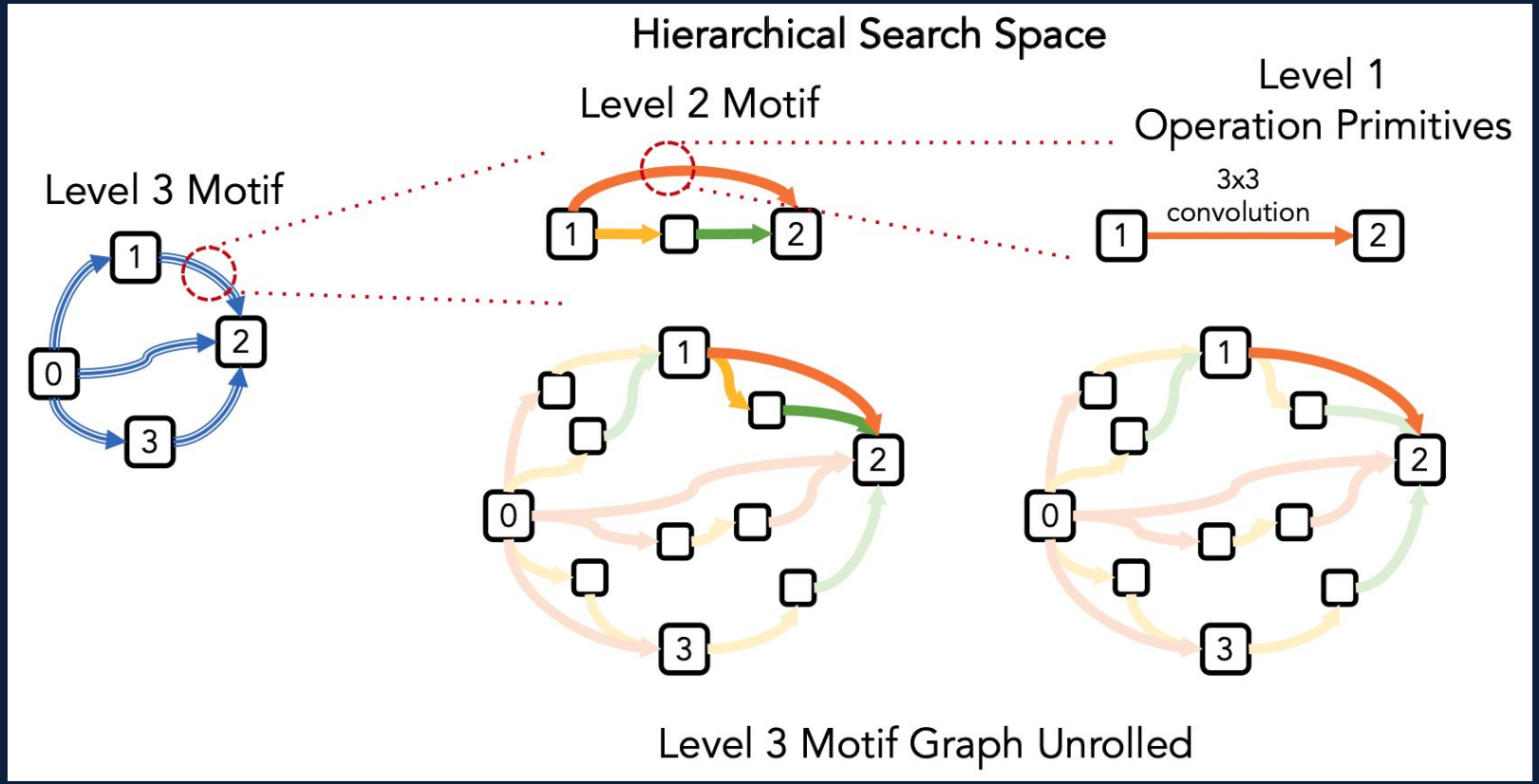
Cell-based search spaces



NASNet (2017)

DARTS (2018)

Hierarchical Search Spaces

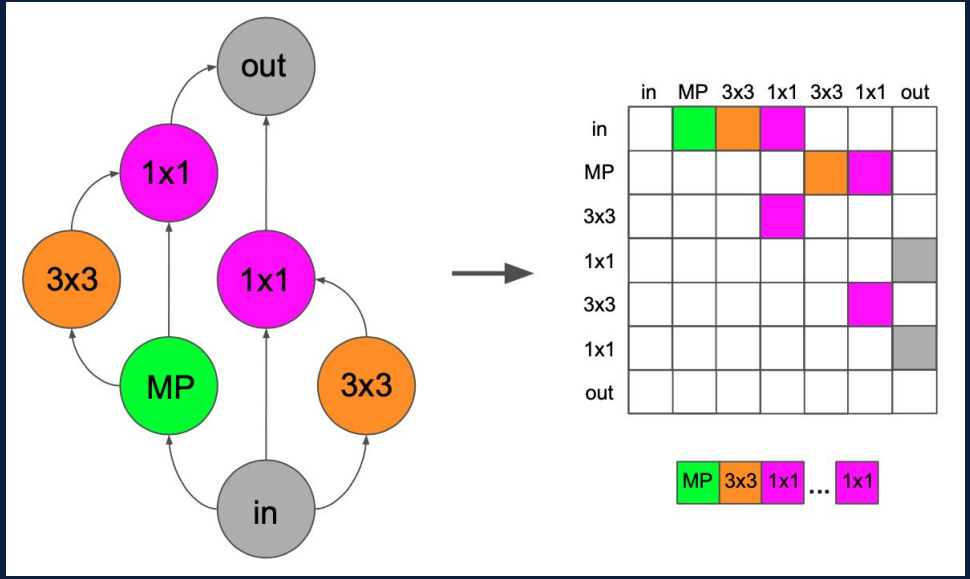


Liu et al. (2017)

Ru et al. (2020)

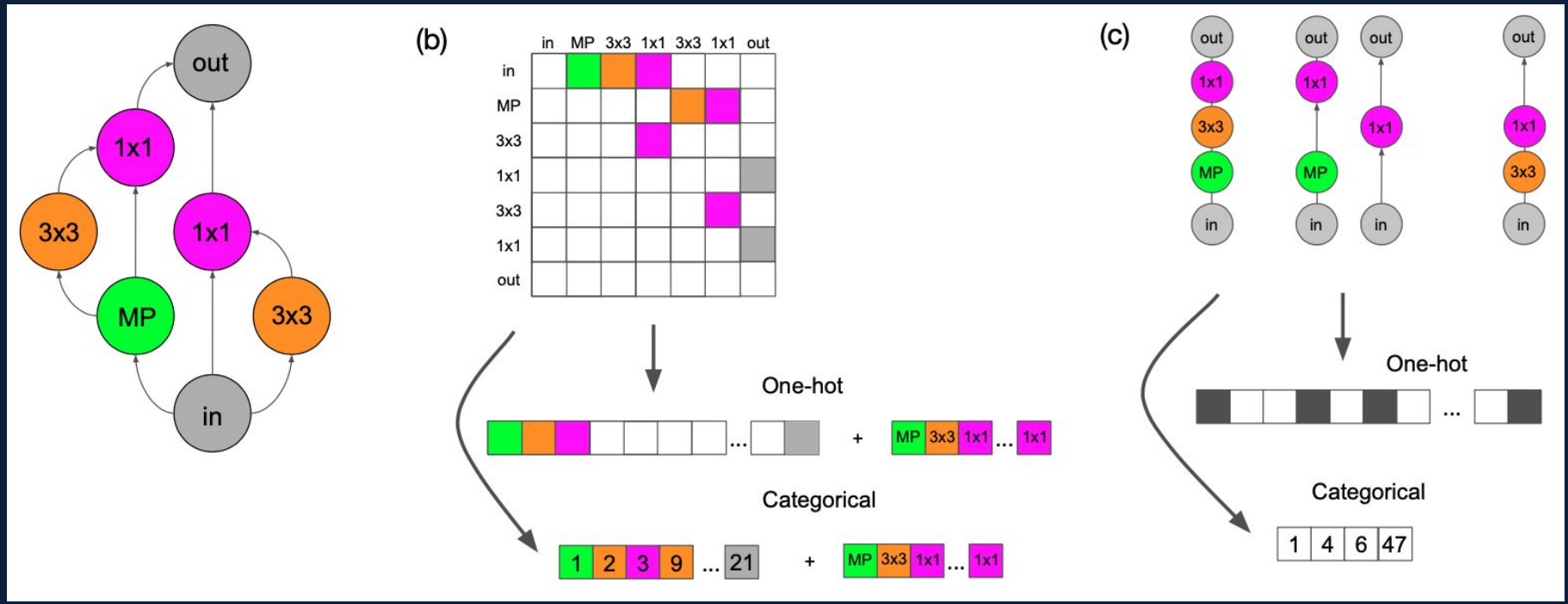
Encodings for NAS

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



White et al. (2020)

Encodings for NAS



White et al. (2020)

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

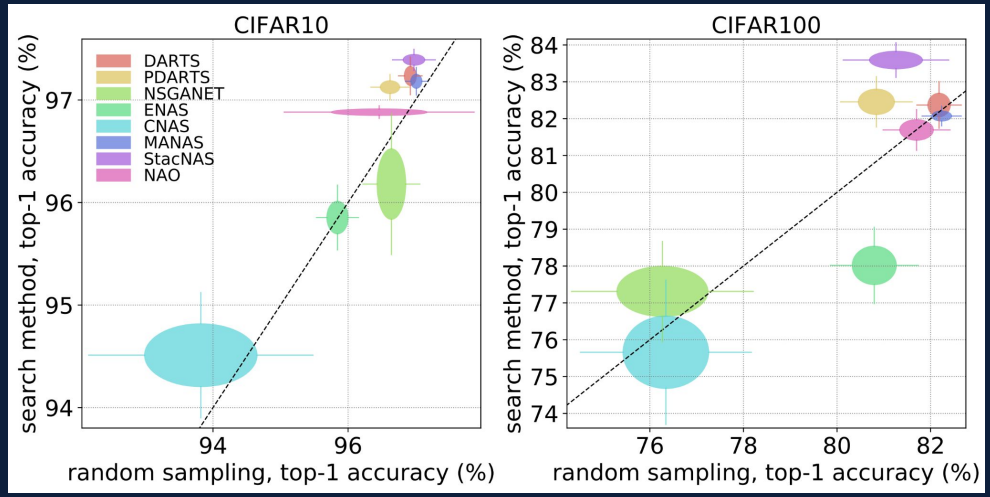
- Introduction
- Search spaces
- Black-box optimization methods
- One-shot methods
- NAS Benchmarks
- Case studies
  - Face Recognition
  - Climate Change
  - Recommender systems

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

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 $i = i + 1$

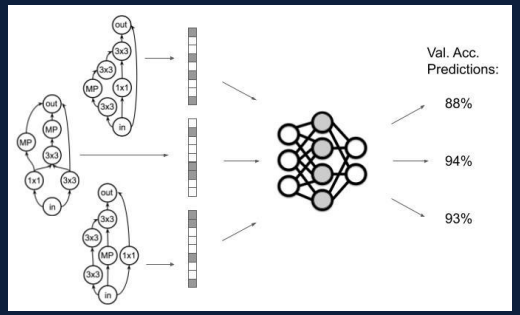
Output: Architecture v_i

[Ottellander et al. 2020]

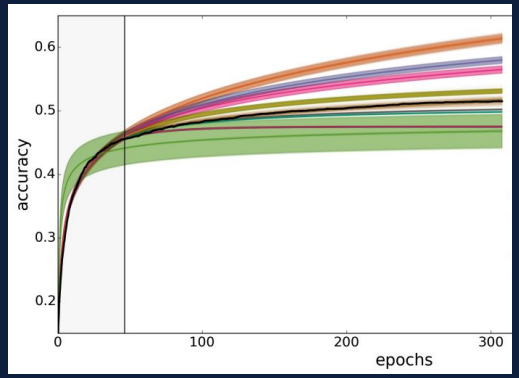
[White et al. 2020]

Performance Predictors

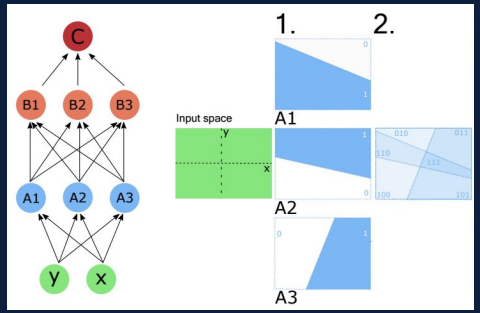
Predict the (relative) accuracy of an architecture, without fully training it.



Model-based



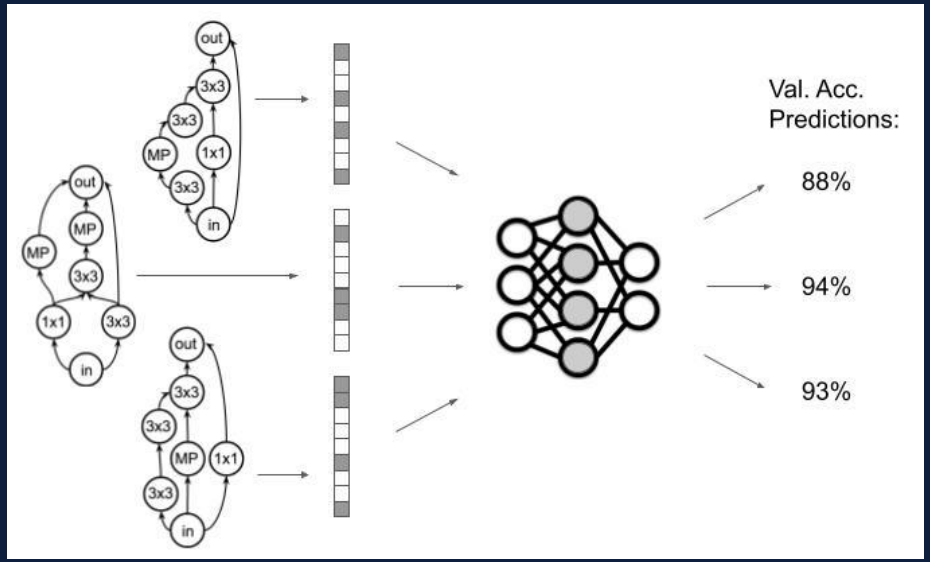
Learning curve extrapolation



Zero-cost proxies

Model-Based Predictors

Train a surrogate model



- 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

“BO + Neural Predictor” Framework

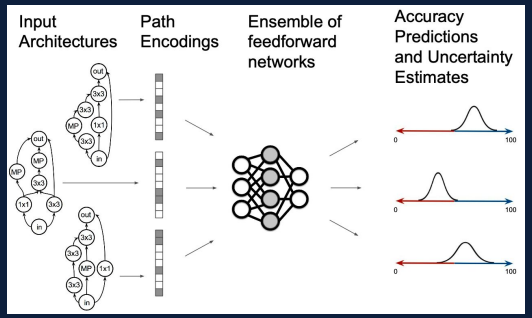
[NASGBO, 2019], [BONAS, 2019], [BANANAS, 2019]

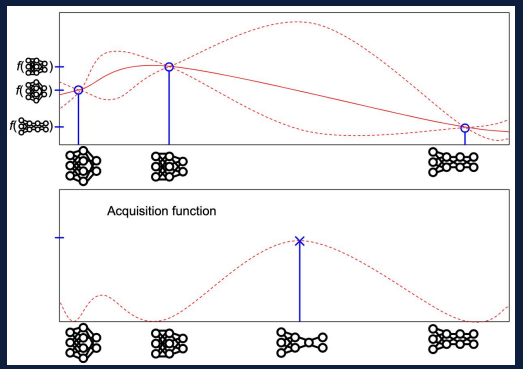
Algorithm 1 BANANAS

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

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

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

BANANAS

Algorithm 1 BANANAS

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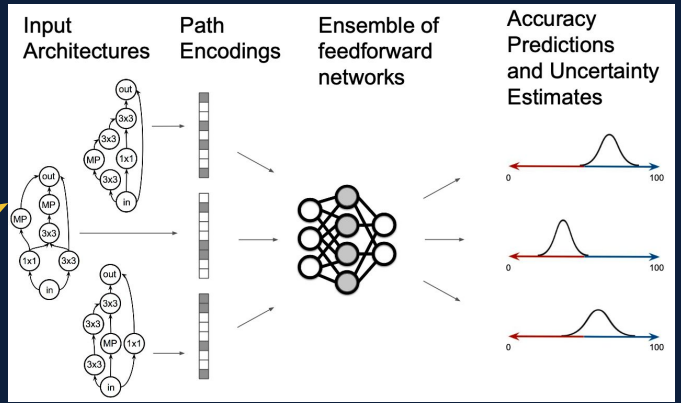


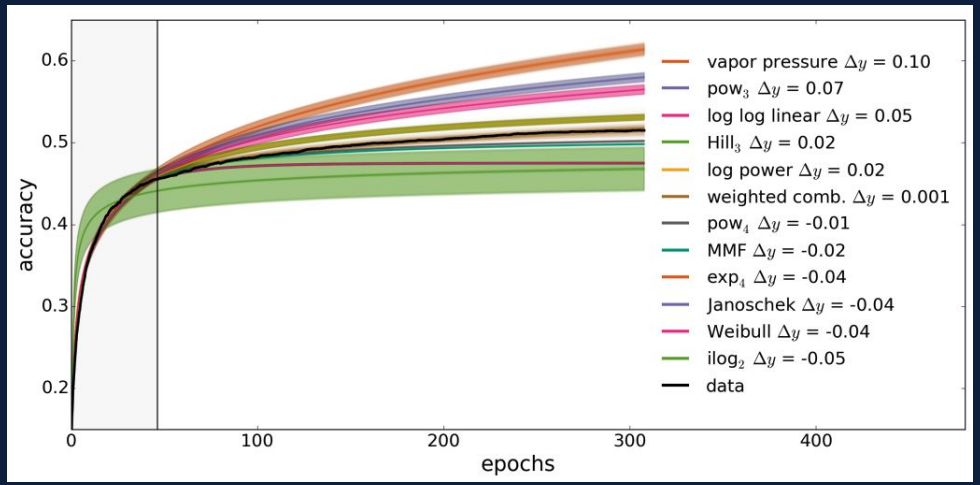
Path encoding, ensemble

Small mutations

Independent Thompson Sampling

BANANAS, 2019

Learning curve based predictors



- Learning curve extrapolation
  - Fit partial learning curve to parametric model [Domhan et al. 2015]
  - Bayesian NN [Klein et al. 2017]
- LCE + Surrogate
  - SVR [Baker et al. 2017]
  - Full LC + Bayesian NN [Klein et al. 2017]

No init time, high query time

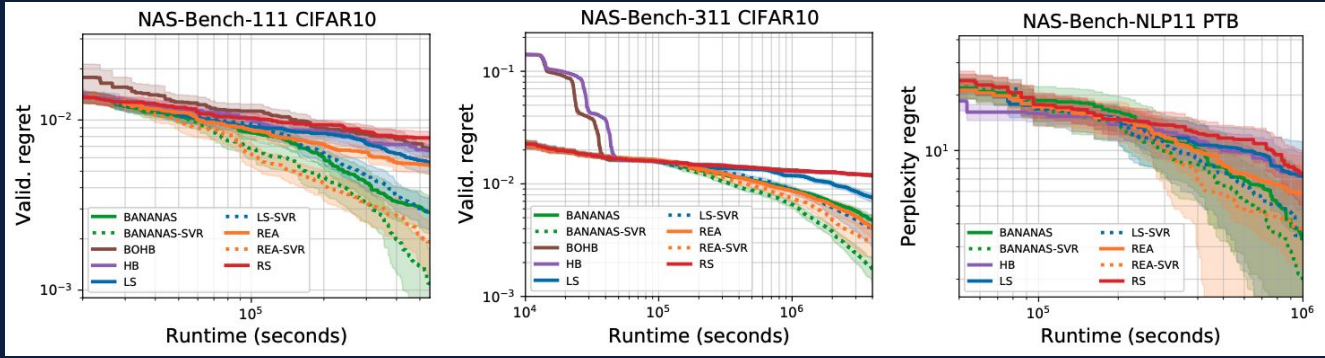
LCE Framework

Algorithm 1 Single-Fidelity Algorithm

```
initialize history
while t < t_max :
  arches = gen_candidates(history)
  accs = train(arches, epoch=E_max)
  history.update(arches, accs)
Return arch with the highest acc
```

Algorithm 2 LCE Framework

```
initialize history
while t < t_max :
  arches = gen_candidates(history)
  accs = train(arches, epoch=E_few)
  sorted_by_pred = LCE(arches, accs)
  arches = sorted_by_pred[:top_n]
  accs = train(arches, epoch=E_max)
  history.update(arches, accs)
Return arch with the highest acc
```

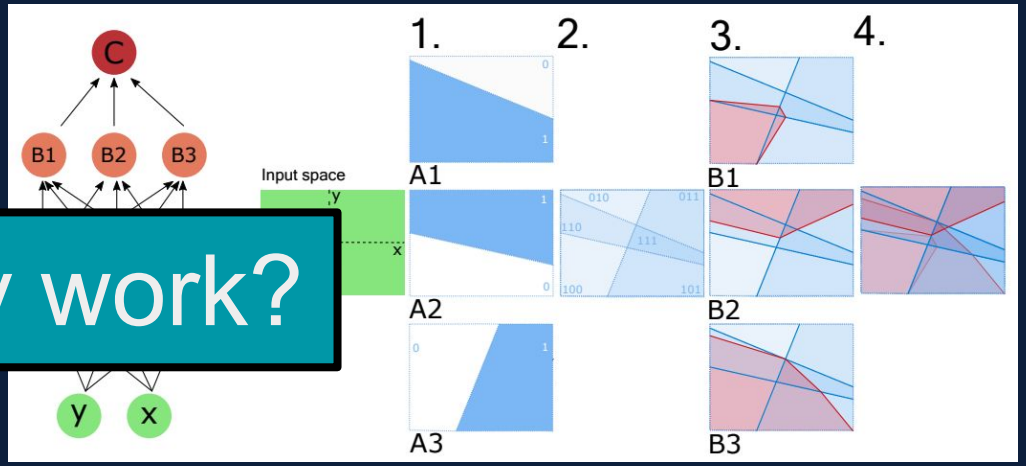


[NAS-Bench-x11, 2021]

Zero-cost proxies

epe-nas [21]	Jacobian
fisher [42]	Pruning-at-init
flops [25]	Baseline
grad-norm [1]	Pruning-at-init
grasp [43]	Pruning-at-init
l2-norm [1]	B
jacov [23]	Ja
nwot [23]	Ja
params [25]	Baseline
plain [1]	Baseline
snip [14]	Pruning-at-init
synflow [39]	Pruning-at-init
zen-score [16]	Piece. Lin.

Do they work?



[Mellor et al. 2020]

Compute an estimate in 5 seconds

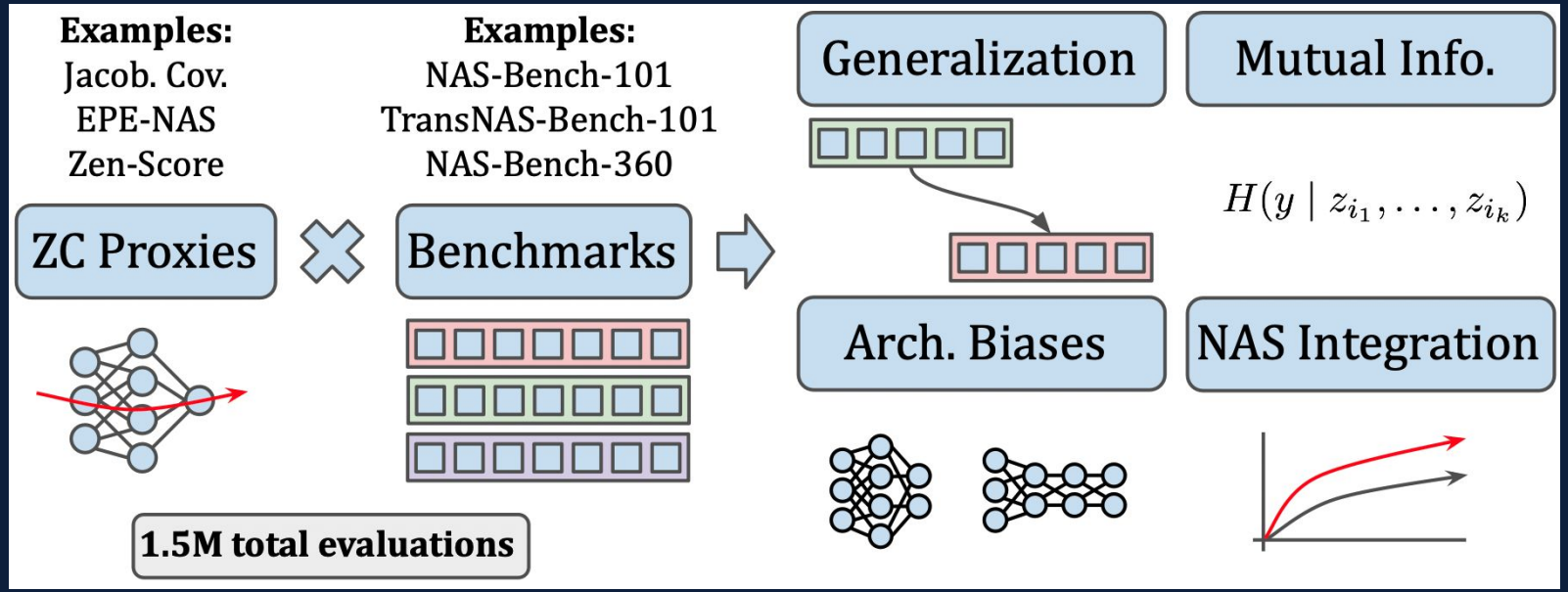
Zero-cost proxies

Table 4: Average ranking of each of the ZC proxies on each search space, and over all search spaces.

	fisher	grad_norm	grasp	jacob_cov	snip	synflow	flops	params
NATS-Bench TSS	6.0	6.0	5.0	4.0	5.67	**1.33**	4.0	4.0
DARTS	4.6	4.2	4.6	4.8	4.6	5.4	4.0	**3.8**
TransNAS-Bench-101	**2.75**	4.5	4.5	7.5	3.0	4.5	4.0	5.25
Overall	4.33	4.75	4.67	5.5	4.33	4.08	**4.0**	4.33

White et al., 2022

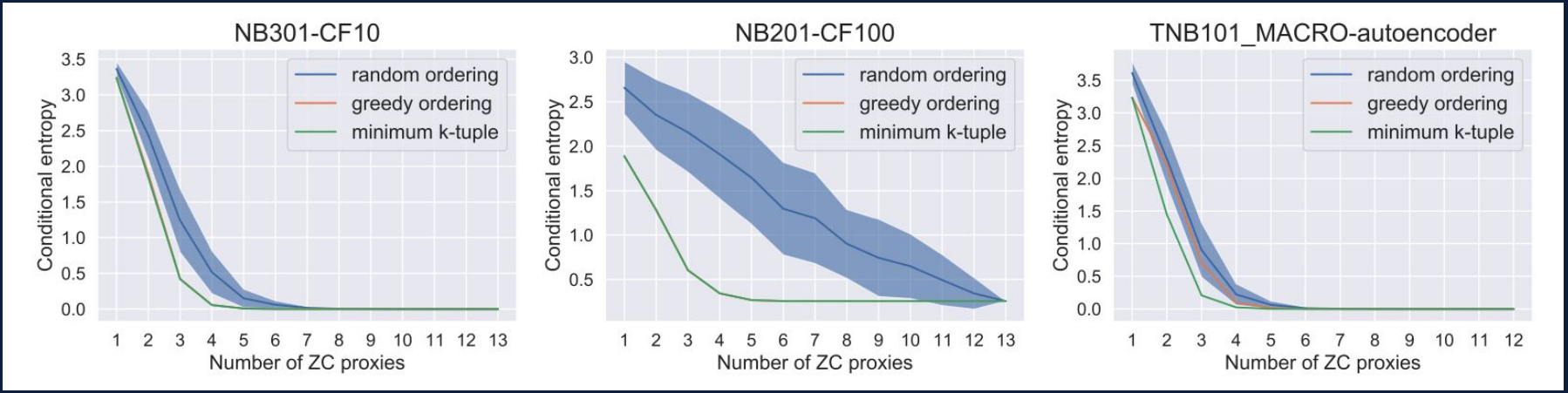
NAS-Bench-Suite-Zero (28 tasks)



NAS-Bench-Suite-Zero, 2022

https://github.com/automl/NASLib/tree/zerocost

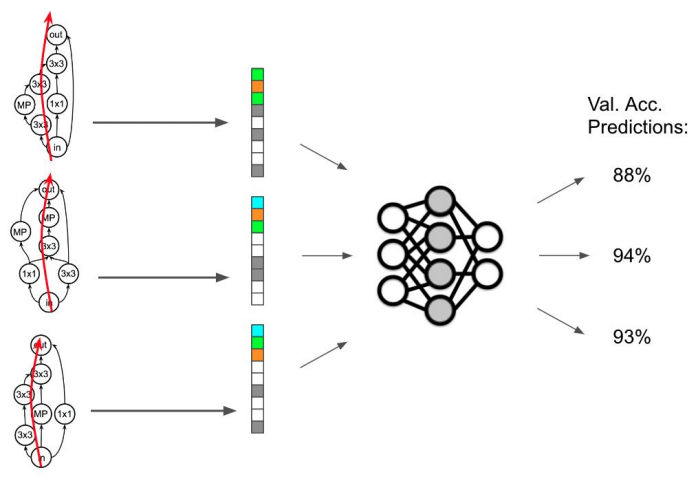
Complementary info in ZC proxies



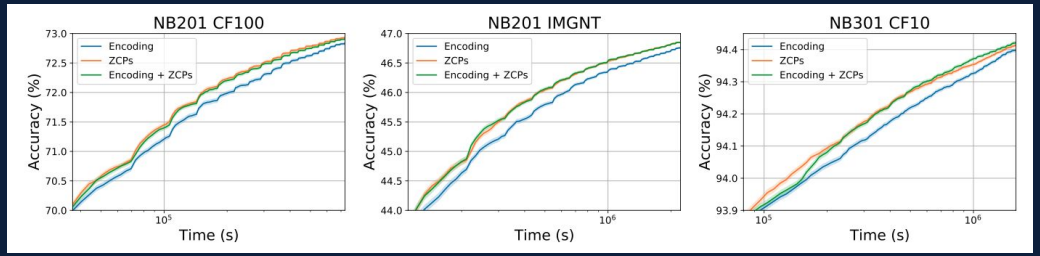
Conditional entropy $H(y \mid z_{i_1}, \ldots, z_{i_k})$ vs. k

NAS-Bench-Suite-Zero, 2022

NAS integration

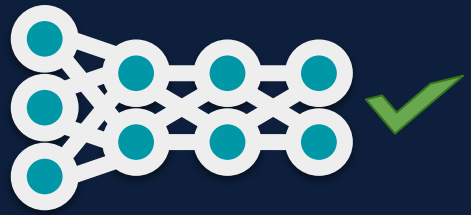


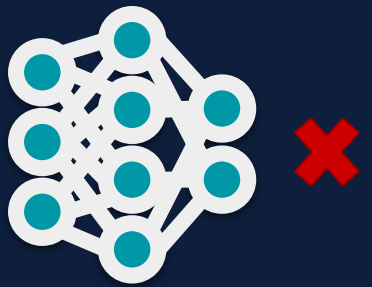
Features Benchmark	Encoding	ZC	Both	% Improvement (ZC)	% Improvement (Both)
NB101-CF10	0.546	0.708	0.718	29.67	31.50
NB201-CF10	0.622	0.905	0.906	45.50	45.66
NB201-CF100	0.640	0.907	0.908	41.71	41.87
NB201-IMGNT	0.683	0.879	0.883	28.70	29.28
NB301-CF10	0.314	0.405	0.465	28.98	48.09
TNB101_MACRO-AUTOENC	0.673	0.831	0.837	23.48	24.37
TNB101_MACRO-JIGSAW	0.809	0.706	0.809	-12.73	0.00
TNB101_MACRO-NORMAL	0.617	0.710	0.716	15.07	16.05
TNB101_MACRO-OBJECT	0.736	0.840	0.843	14.13	14.54
TNB101_MACRO-ROOM	0.683	0.589	0.707	-13.76	3.51
TNB101_MACRO-SCENE	0.832	0.891	0.899	7.09	8.05
TNB101_MACRO-SEGMENT	0.900	0.807	0.876	-10.33	-2.67
TNB101_MICRO-AUTOENC	0.714	0.754	0.803	5.60	12.46
TNB101_MICRO-JIGSAW	0.585	0.730	0.743	24.79	27.01
TNB101_MICRO-NORMAL	0.657	0.801	0.809	21.92	23.14
TNB101_MICRO-OBJECT	0.637	0.733	0.752	15.07	18.05
TNB101_MICRO-ROOM	0.582	0.843	0.844	44.85	45.02
TNB101_MICRO-SCENE	0.710	0.849	0.866	19.58	21.97
TNB101_MICRO-SEGMENT	0.767	0.886	0.897	15.51	16.95



[NAS-Bench-Suite-Zero, 2022]

Removing biases in ZC proxies



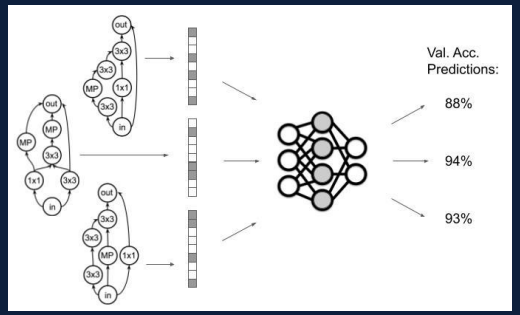


$$f'(a) = f(a) \cdot \frac{1}{b(a) + C}$$

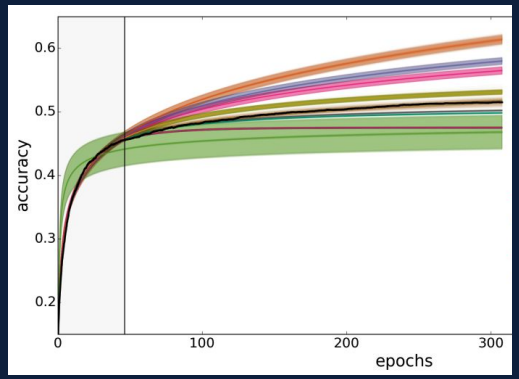
ZC proxy	dataset	bias metric	original bias	original perf.	new bias	new perf.	strategy
l2-norm	NB201-CF10	conv:pool	0.87	0.42	0.00	0.10	minimize
					0.37	0.11	equalize
					0.70	0.44	performance
nwot	NB301-CF10	conv:pool	0.78	0.49	0.00	0.03	minimize
					0.29	0.14	equalize
					0.78	0.49	performance
synflow	NB201-CF100	cell size	0.57	0.68	0.01	0.64	minimize
					0.35	0.71	equalize
					0.35	0.71	performance
synflow	NB201-IM	cell size	0.58	0.76	0.01	0.62	minimize
					0.43	0.76	equalize
					0.46	0.76	performance
flops	NB301-CF10	num. skip	-0.35	0.43	-0.01	0.06	minimize
					0.12	-0.05	equalize
					-0.35	0.43	performance

NAS-Bench-Suite-Zero, 2022

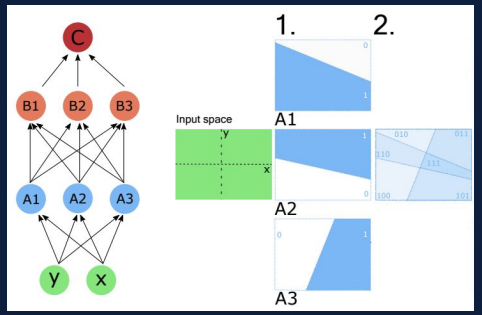
Performance predictor families



Model-based

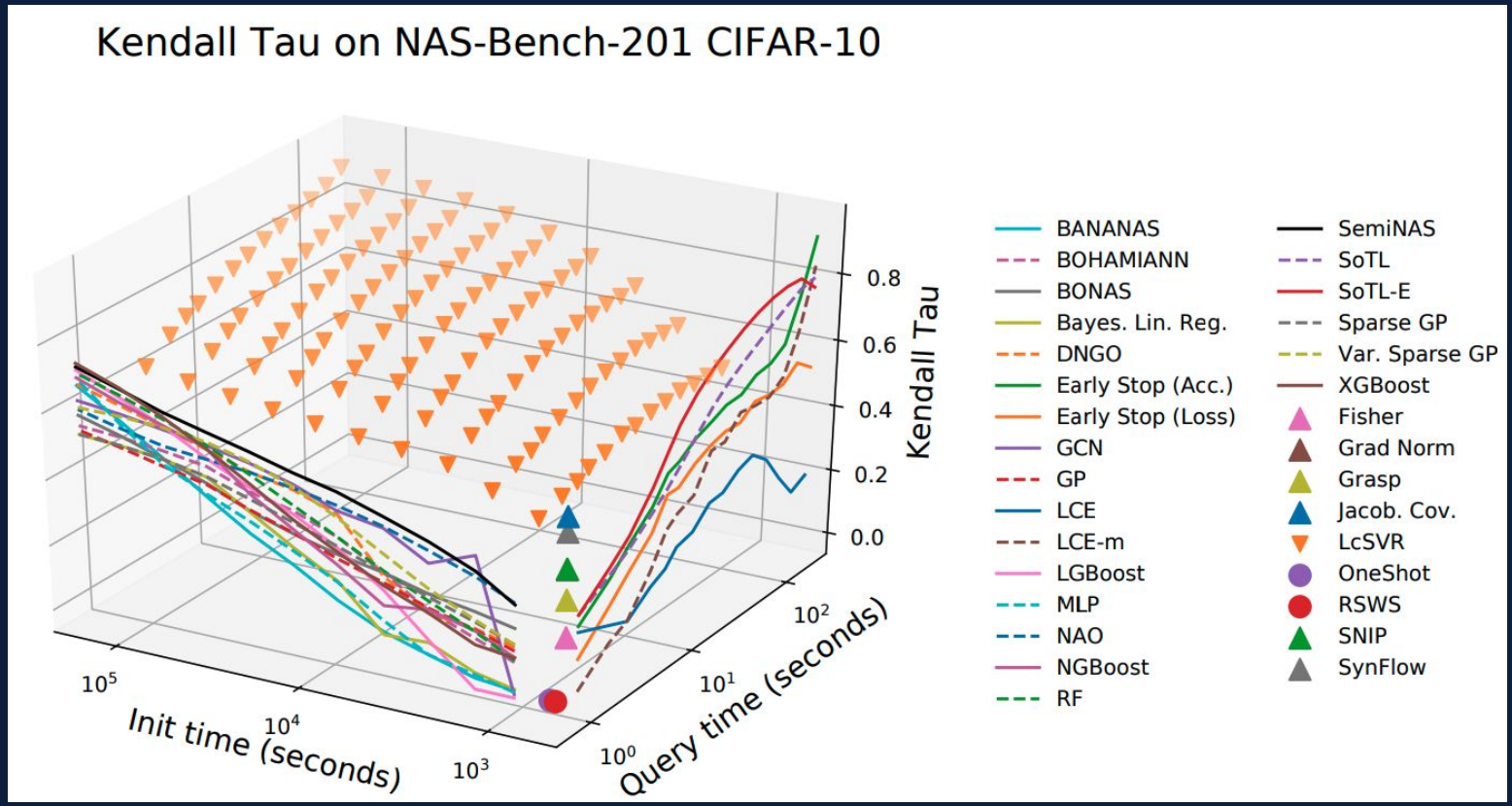


Learning curve extrapolation

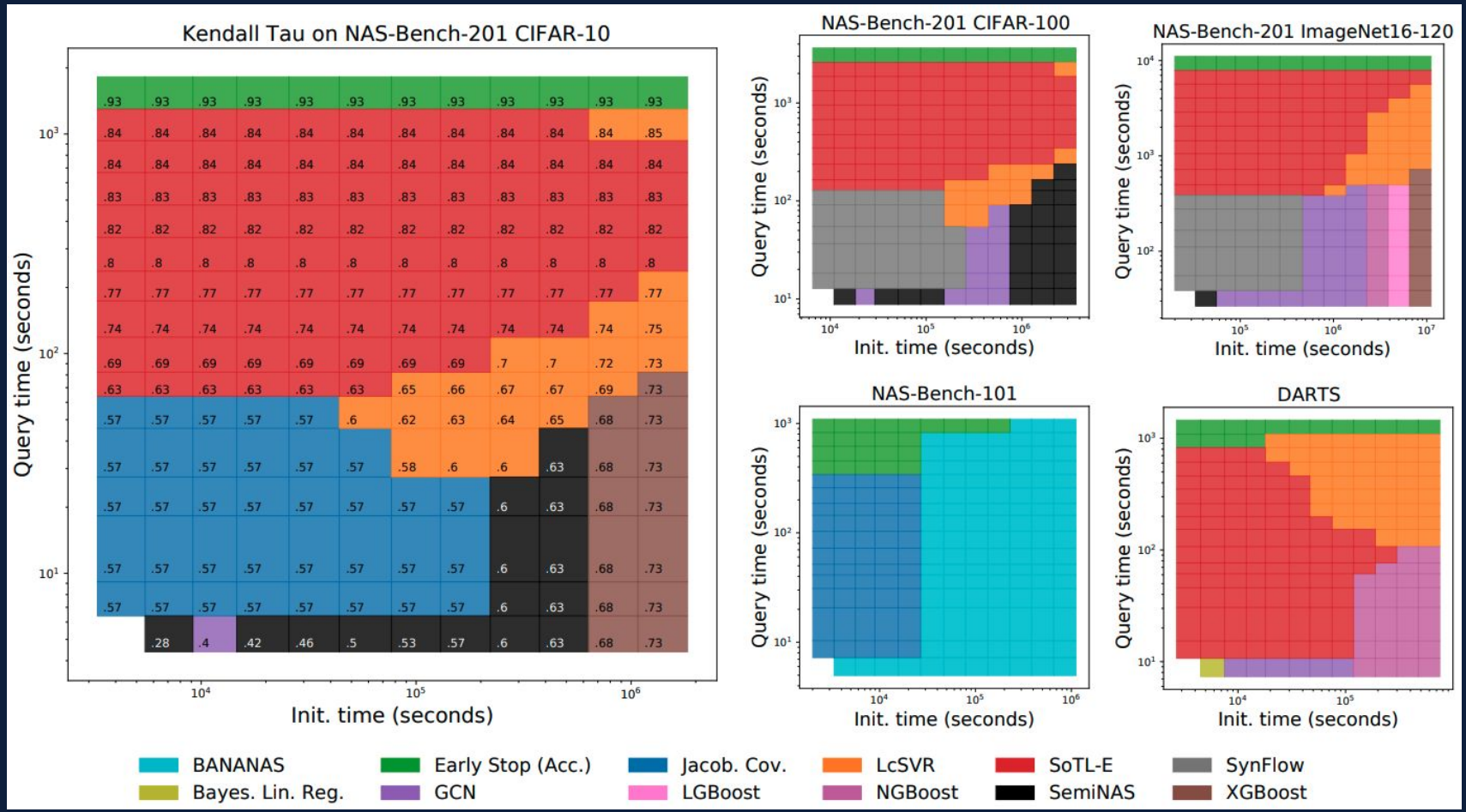


Zero-cost proxies

Performance predictors

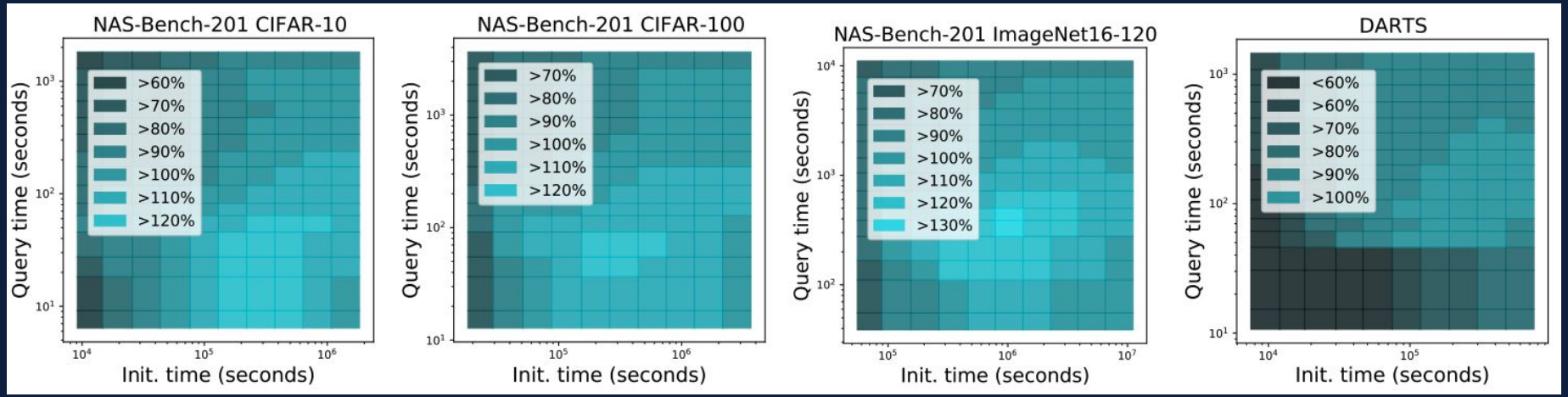


White et al., 2021


Kendall Tau on NAS-Bench-201 CIFAR-10
Query time (seconds)
Init. time (seconds)
NAS-Bench-201 CIFAR-100
NAS-Bench-201 ImageNet16-120
NAS-Bench-101
DARTS
BANANAS
Bayes. Lin. Reg.
Early Stop (Acc.)
GCN
Jacob. Cov.
LGBoost
LcSVR
NGBoost
SoTL-E
SemiNAS
SynFlow
XGBoost

OMNI: The Omnipotent Predictor

Combine best predictors from each family

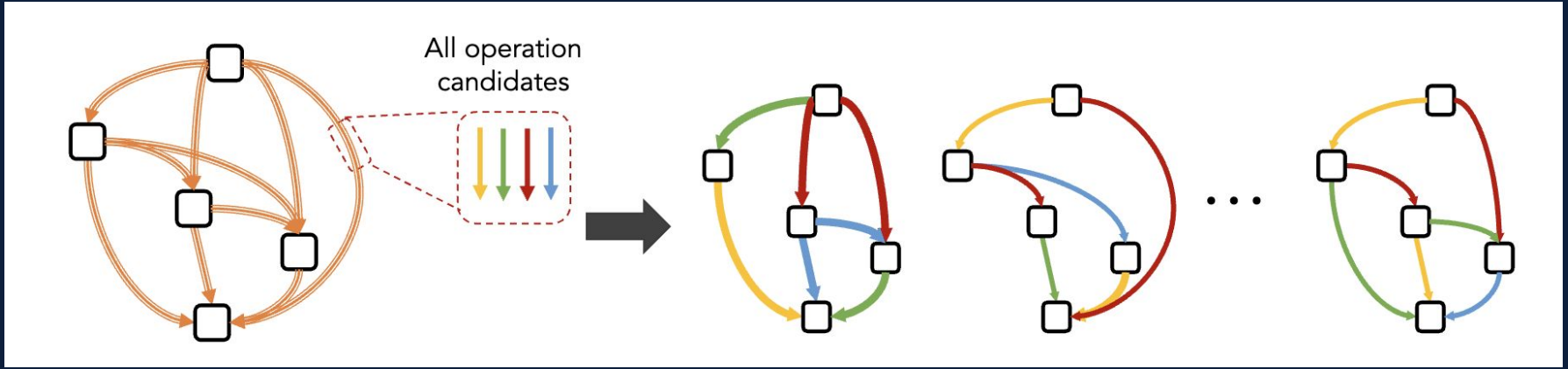


White et al., 2021

Roadmap

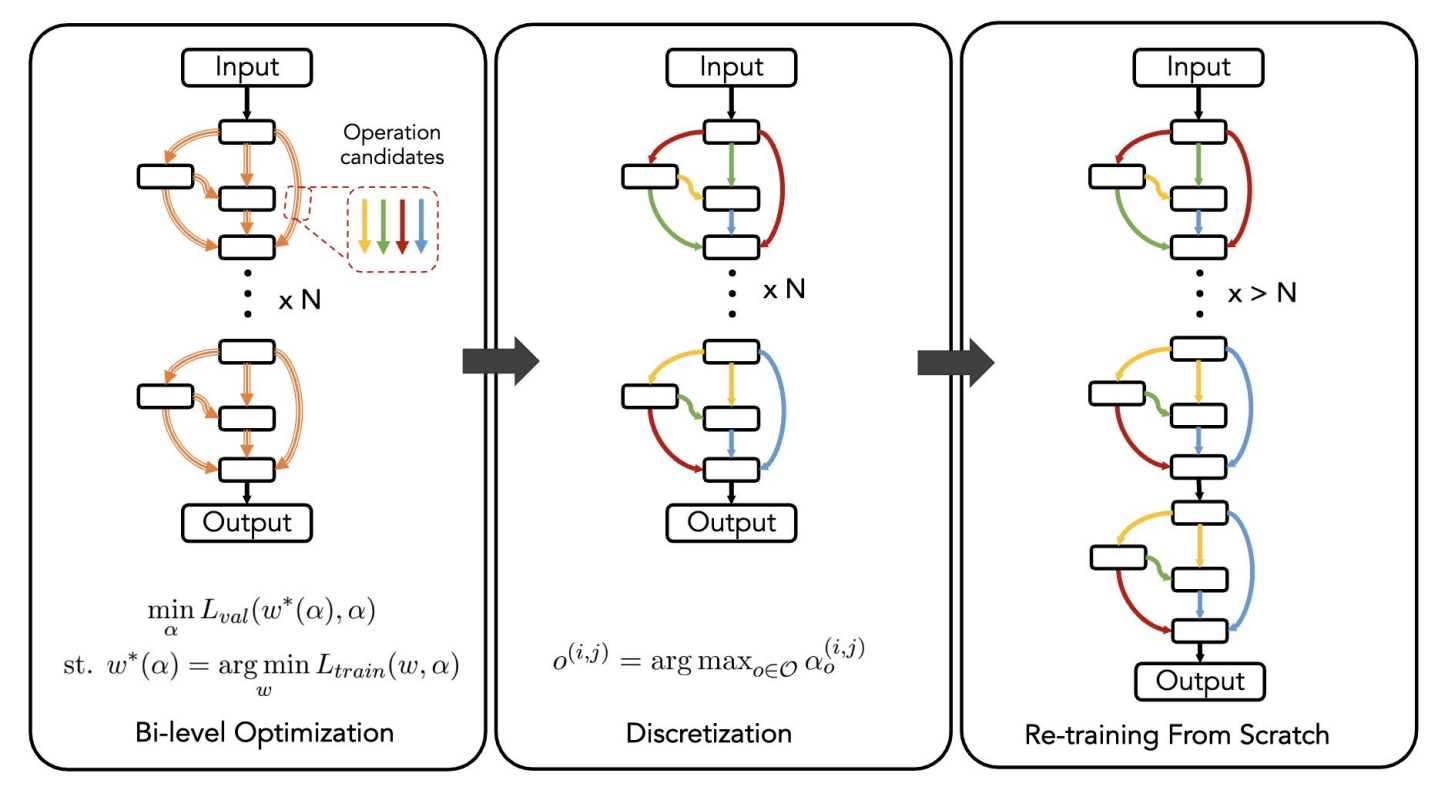
- Introduction
- Search spaces
- Black-box optimization methods
- One-shot methods
- NAS Benchmarks
- Case studies
  - Face Recognition
  - Climate Change
  - Recommender systems

One-shot methods



Bender et al., 2018

DARTS



DARTS, 2018

DARTS-PT

Evaluate operation strength in terms of contribution to the supernet's performance

Algorithm 1: Perturbation-based Architecture Selection

Input: A pretrained supernet S, Set of edges $\mathcal{E}$ from S, Set of nodes $\mathcal{N}$ from S
Result: Set of selected operations $\{o_e^*\}_{e \in \mathcal{E}}$
while $|\mathcal{E}| > 0$ **do**
    randomly select an edge $e \in \mathcal{E}$ (and remove it from $\mathcal{E}$);
    forall *operation* o *on edge* e **do**
        evaluate the validation accuracy of S when o is removed ($ACC_{\backslash o}$);
    end
    select the best operation for e: $o_e^* \leftarrow \arg\min_o ACC_{\backslash o}$;
    discretize edge e to o_e^* and tune the remaining supernet for a few epochs;
end

DARTS-PT, 2021

Roadmap

- Introduction
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- One-shot methods
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- Case studies
  - Face Recognition
  - Climate Change
  - Recommender systems

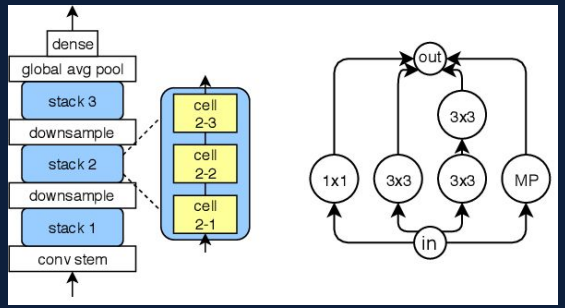
Tables of results

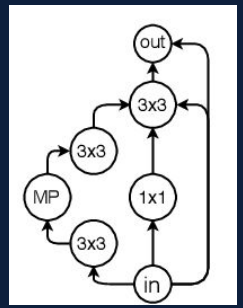
- Different epochs
- Different hardware
- Few trials

Architecture	Test Error (%)	Params (M)	Search Cost (GPU days)	Search Method
DenseNet-BC (Huang et al., 2017)	3.46	25.6	-	manual
NASNet-A (Zoph et al., 2018)	2.65	3.3	2000	RL
AmoebaNet-A (Real et	3.34 ± 0.06	3.2	3150	evolution
AmoebaNet-B (Real et	2.55 ± 0.05	2.8	3150	evolution
PNAS (Liu et al., 2018)*	3.41 ± 0.09	3	225	SMBO
ENAS (Pham et al., 2018)	2.89		0.5	RL
NAONet (Luo et al., 2018)	3.53		0.4	NAO
SNAS (moderate) (Xie et al., 20	85 ± 0.0	8	1.5	gradient
GDAS (Dong & Yang, 2019)	2.93	3.4	0.3	gradient
BayesNAS (Zhou et al., 2019)		3.4	0.2	gradient
ProxylessNAS (Cai et al., 2019)†		5.7	4.0	gradient
NASP (Yao et al., 2020)	2	3.3	0.1	gradient
P-DARTS (Chen et al., 2019)		3.4	0.3	gradient
PC-DARTS (Xu et al., 2020)	± 0	3.6	0.1	gradient
R-DARTS (L2) Zela et al. (2020	95 ± 0.2		1.6	gradient
DARTS (Liu et al., 2019)	3.00 ± 0.14		0.4	gradient
SDARTS-RS (Chen & Hsie	2.67 ± 0.03		0.4	gradient
SGAS (Cri 1. avg) (Li et	2.66 ± 0.24	3	0.25	gradient
DARTS+PT (avg)*	2.61 ± 0.08	3.0	0.8‡	gradient
DARTS+PT (best)	2.48	3.3	0.8‡	gradient
SDARTS-RS+PT (avg)*	2.54 ± 0.10	3.3	0.8‡	gradient
SDARTS-RS+PT (best)	2.44	3.2	0.8‡	gradient
SGAS+PT (Crit.1 avg)*	2.56 ± 0.10	3.9	0.29‡	gradient
SGAS+PT (Crit.1 best)	2.46	3.9	0.29‡	gradient

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)
```

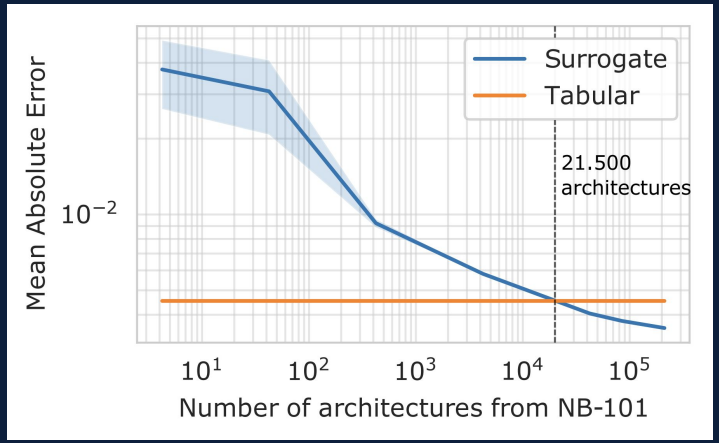
[NAS-Bench-101 (2019)]

NAS Benchmarks

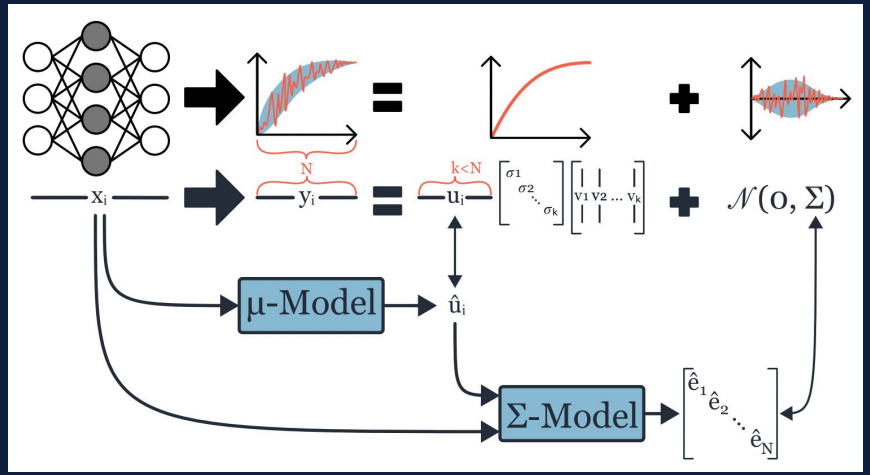
		Queryable						
Benchmark	**Size**	**Tab.**	**Surr.**	**LCs**	**Macro**	**One-Shot**	**Task**	**#Tasks**
NAS-Bench-101	423k	✓				✗	Image class.	1
NATS-Bench-TSS (NAS-Bench-201)	6k	✓		✓		✓	Image class.	3
NATS-Bench-SSS	32k	✓		✓	✓	✓	Image class.	3
NAS-Bench-NLP	$> 10^{53}$			✓		✗	NLP	1
NAS-Bench-1Shot1	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

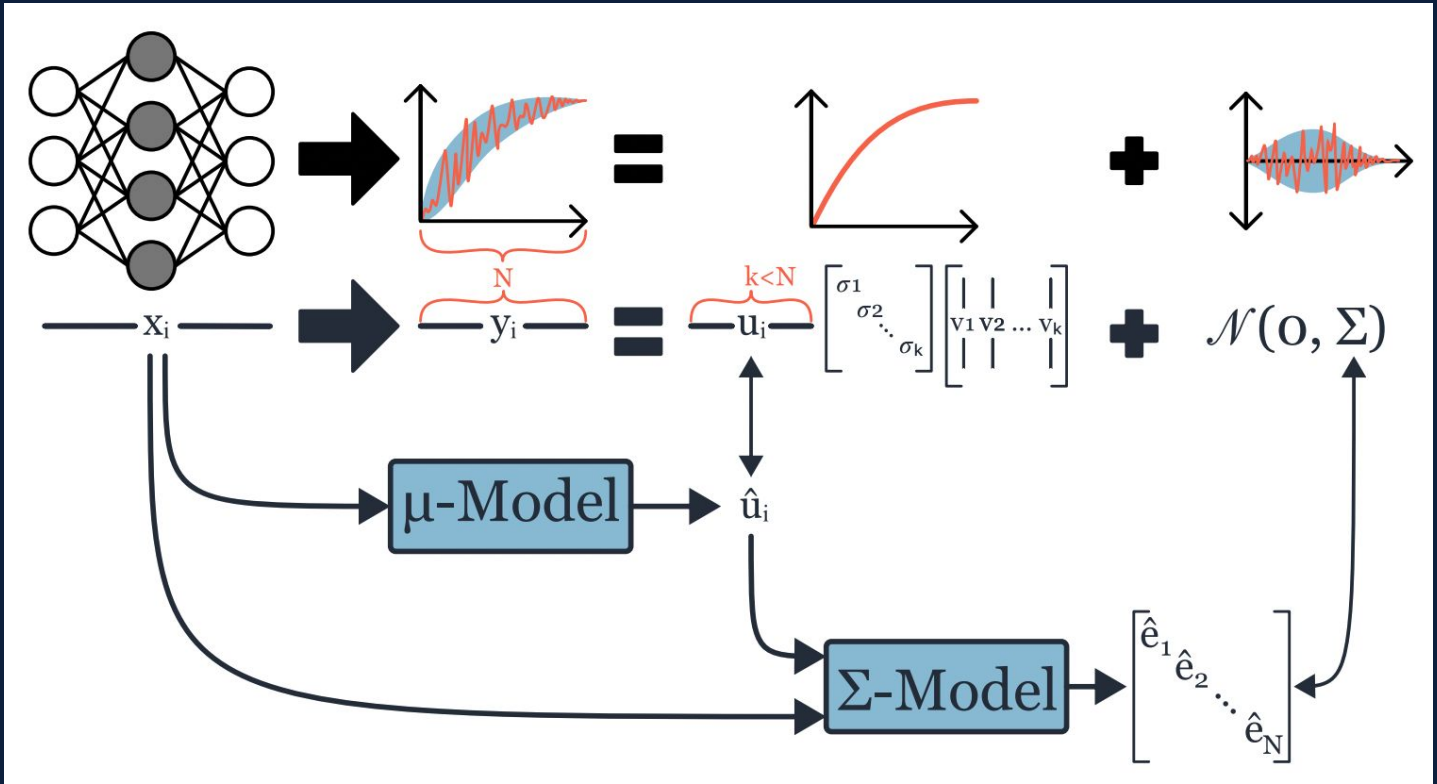


Surr-NAS-Bench (2020)



NAS-Bench-x11 (2021)

NAS-Bench-x11

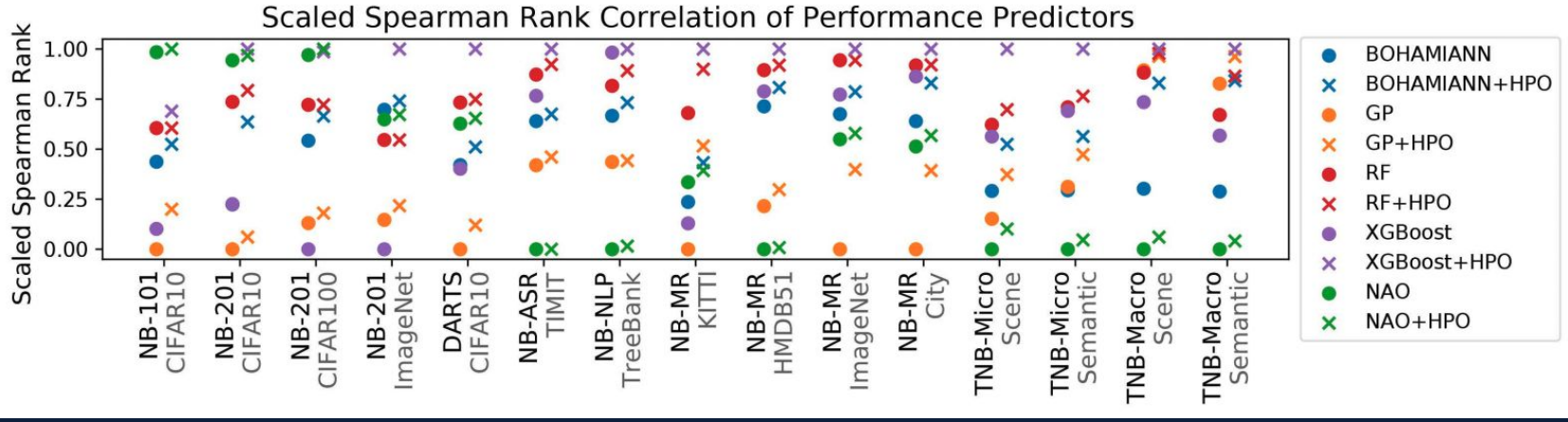


NAS-Bench-x11 (2021)

NAS-Bench-Suite (25 tasks)

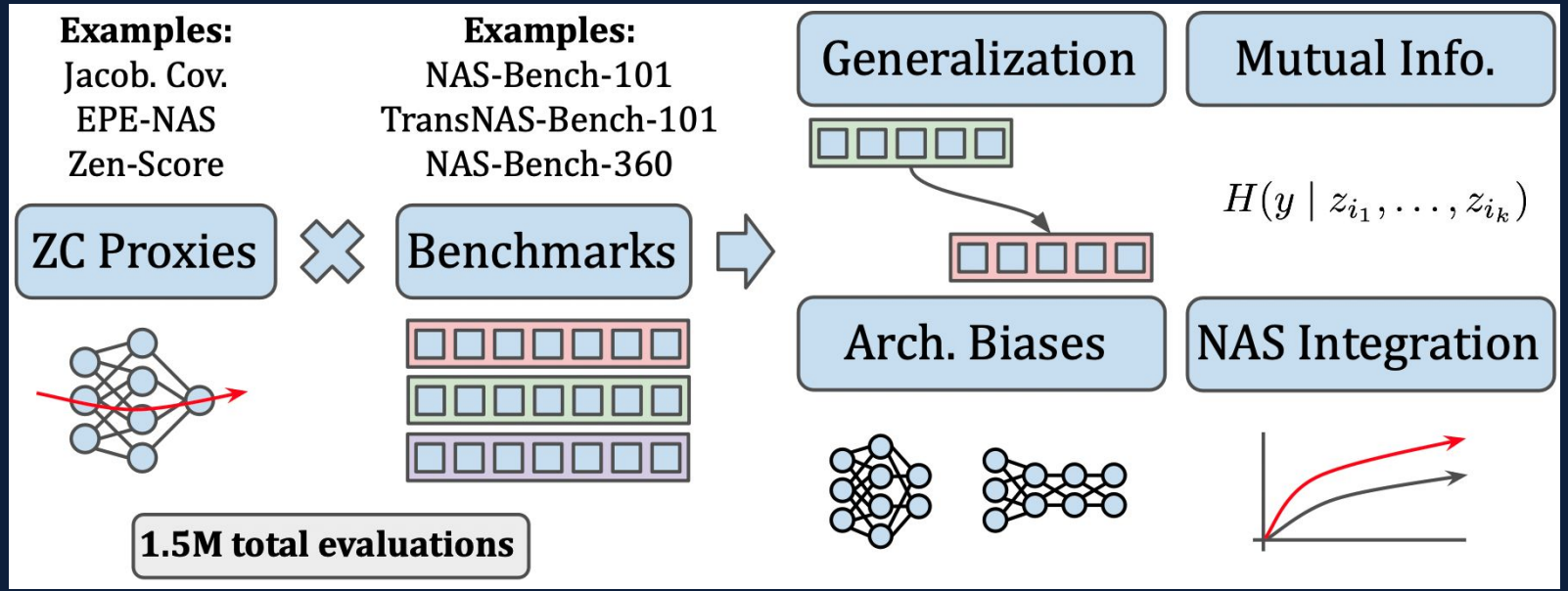
	NAS Algorithms					Performance Predictors				
	RS	RE	BANANAS	LS	NPENAS	GP	BOHAM.	RF	XGB	NAO
Avg.Rank, 101&201	4.50	3.00	3.50	**1.50**	2.50	4.67	2.83	2.17	4.17	**1.17**
Avg. Rank, non-101&201	3.06	**2.11**	2.83	3.13	3.87	4.08	3.06	**1.33**	2.46	4.08

- 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

NAS-Bench-Suite-Zero (28 tasks)



NAS-Bench-Suite-Zero, 2022

https://github.com/automl/NASLib/tree/zerocost

Roadmap

- Introduction
- Search spaces
- Black-box optimization methods
- One-shot methods
- NAS Benchmarks
- Case studies
  - Face Recognition
  - Climate Change
  - Recommender systems

Face recognition

1. **For one-to-one matching, the team saw higher rates of false positives for Asian and African American faces relative to images of Caucasians.** The differentials often ranged from a factor of 10 to 100 times, depending on the individual algorithm. False positives might present a security concern to the system owner, as they may allow access to impostors.
2. **Among U.S.-developed algorithms, there were similar high rates of false positives in one-to-one matching for Asians, African Americans and native groups** (which include Native American, American Indian, Alaskan Indian and Pacific Islanders). The American Indian demographic had the highest rates of false positives.

'The Computer Got It Wrong': How Facial Recognition Led To False Arrest Of Black Man

June 24, 2020 · 8:00 AM ET

BOBBY ALLYN

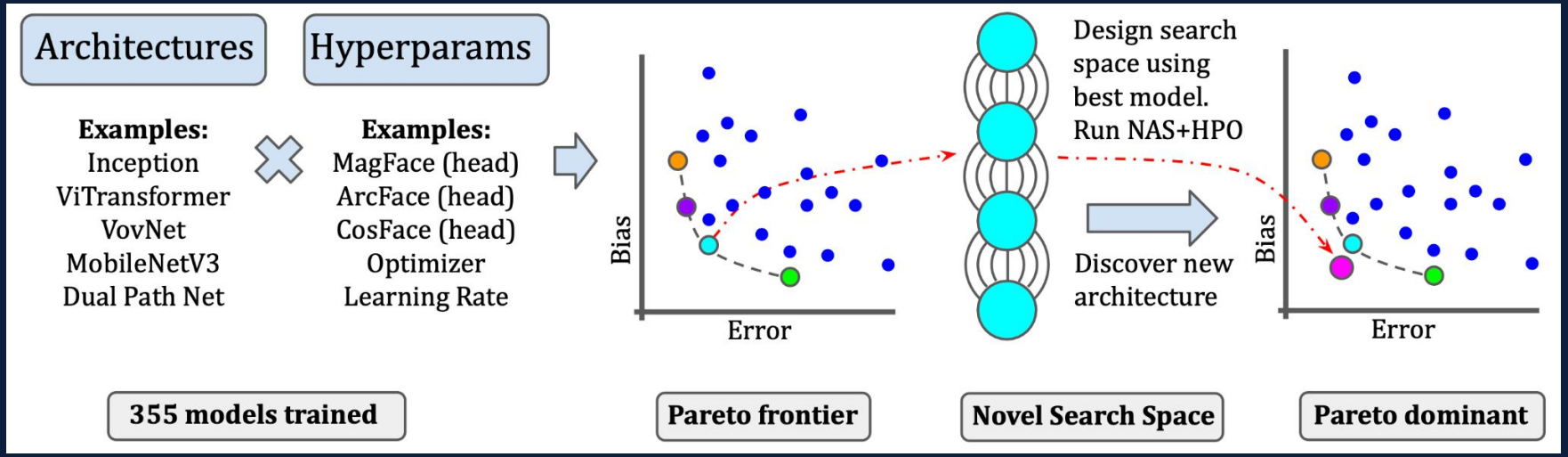
A US government study confirms most face recognition systems are racist

by Karen Hao December 20, 2019

A U.S. Customs and Border Protection officer helps a passenger navigate a facial recognition kiosk at the airport.
DAVID J. PHILLIP/AP

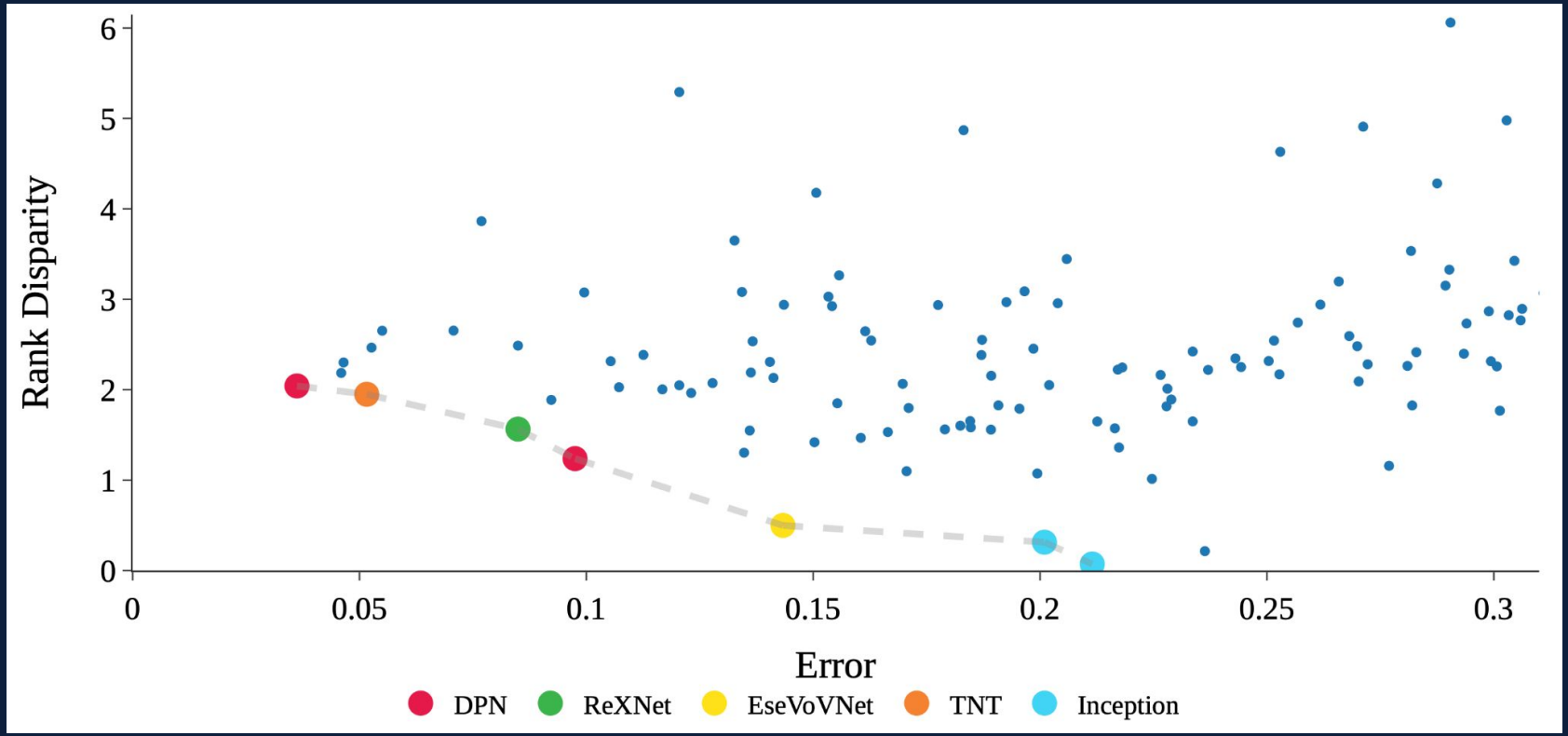
https://www.nist.gov/news-events/news/2019/12/nist-study-evaluates-effects-race-age-sex-face-recognition-software

Face recognition

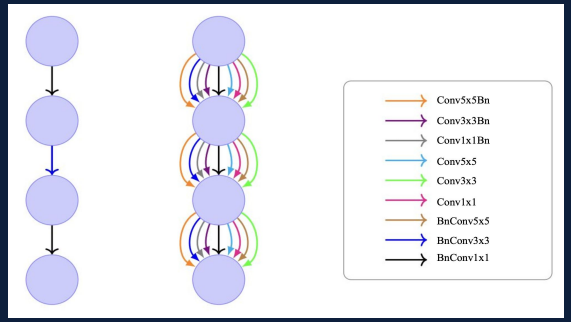


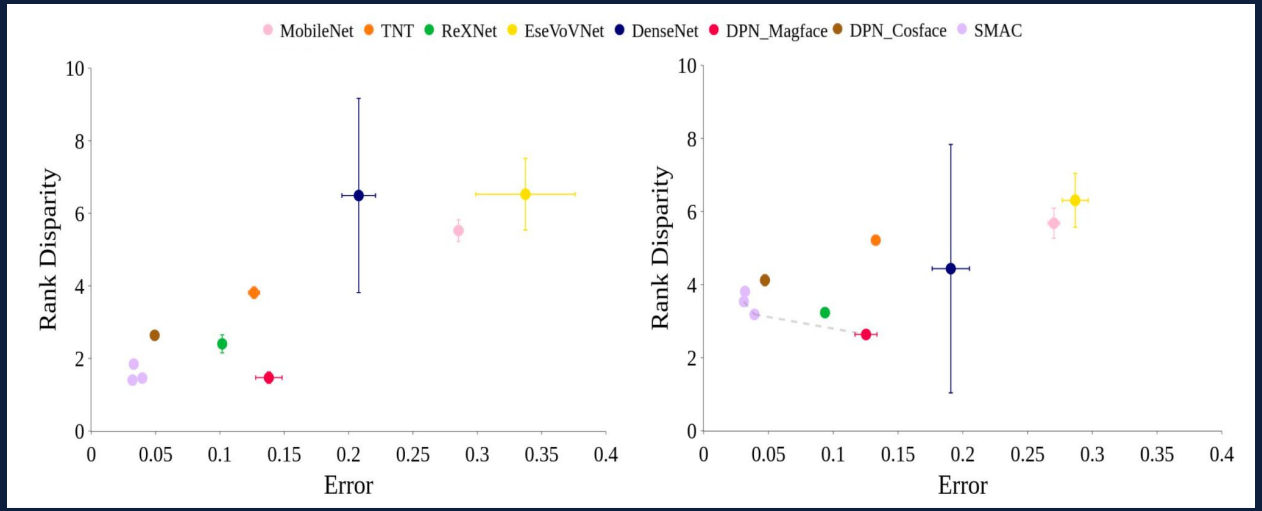
Sukthanker et al., 2022

Face recognition

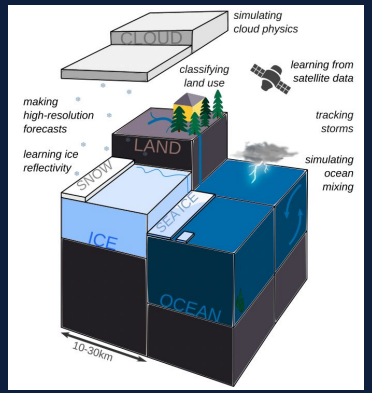


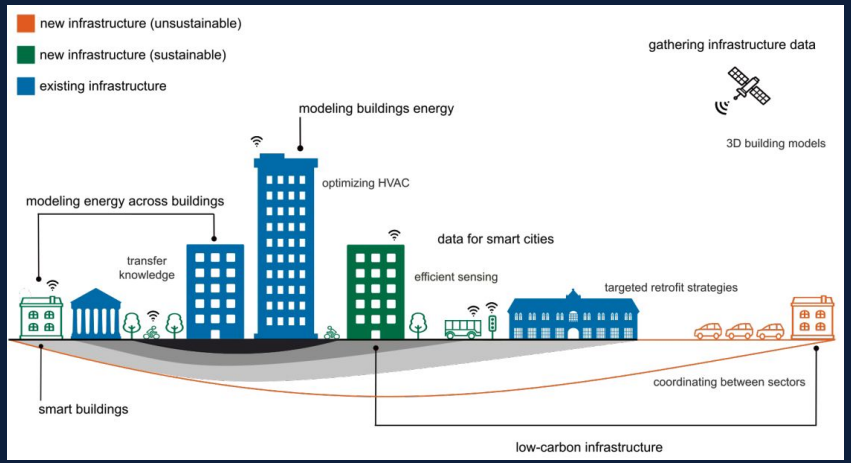
Face recognition

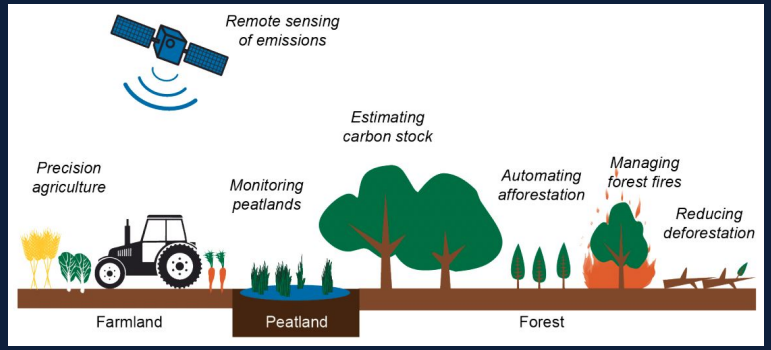




Tackling Climate Change with Machine Learning

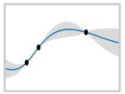
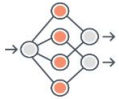






Rolnick et al., 2018

Climate Change AutoML

AutoML Methods	CCAI Benchmarks	Metrics of Interest
 Hyperparameter Optimization **(Optuna)**	 ClimART (**CA**)	Accuracy, Inference Latency
 Neural Architecture Search **(SMAC3)**	 Open Catalyst Project (**OC20**)	Mean Absolute Error Between Energies
	 Wind Power Forecasting (**SDWPF**)	Average Accuracy Across Turbines

Tu et al., 2022

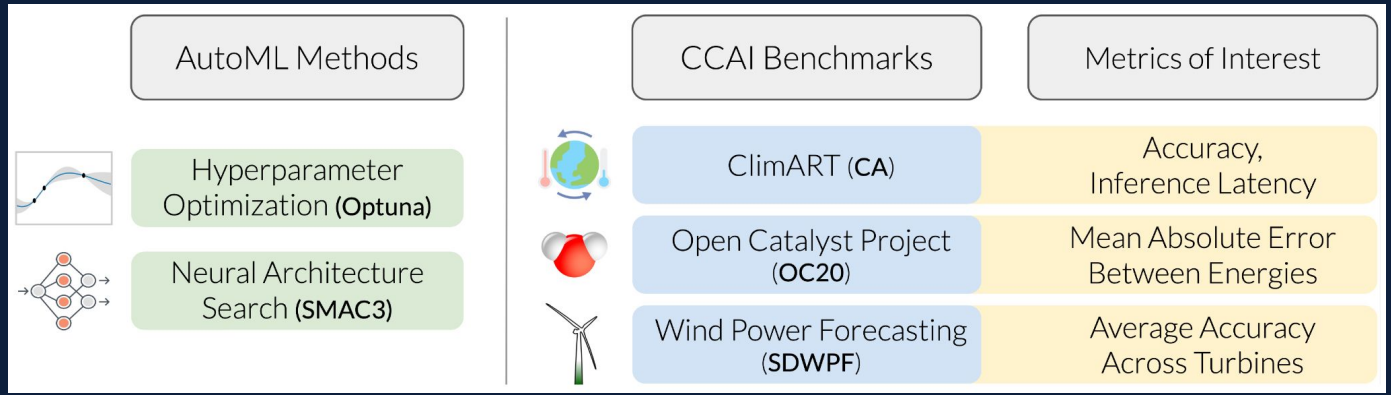
Climate Change AutoML

Dataset	Type	Base Model	Metric	Perf. human	Perf. AutoML	improv. %	search time
ClimART	NAS	Various	RMSE (W/m^2)	1.829	1.669	8.7%	12 GPU hrs
ClimART	HPO	CNN	RMSE (W/m^2)	1.829	1.538	15.9%	54 GPU hrs
SDWPF	NAS	BERT-based	RMSE+MAE (kW)	45.246	45.178	0.15%	26 GPU hrs
SDWPF	HPO	BERT-based	RMSE+MAE (kW)	45.246	45.329	-0.08%*	42 GPU hrs
SDWPF	HPO	GRU+GBDT	RMSE+MAE (kW)	45.074	45.074	0%	50 GPU hrs
OC20	HPO	Graphormer	MAE (eV)	0.399	0.396	0.65%	24 GPU hrs

Tu et al., 2022

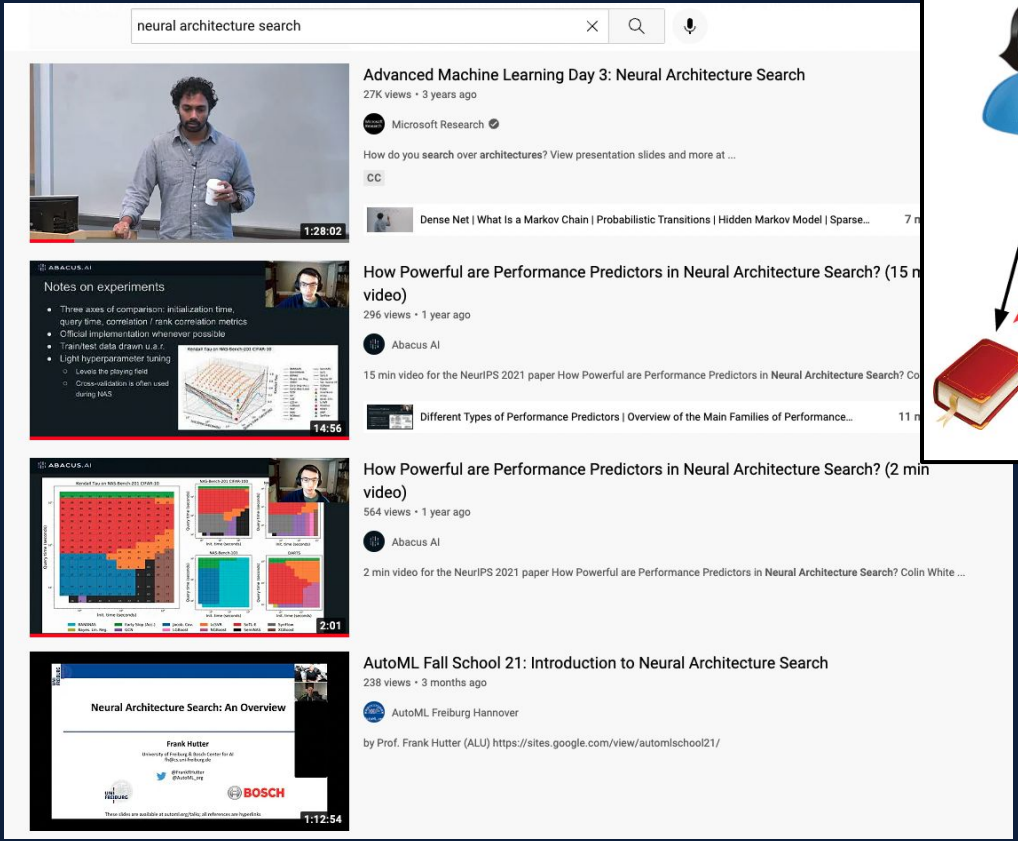
A Call to Action

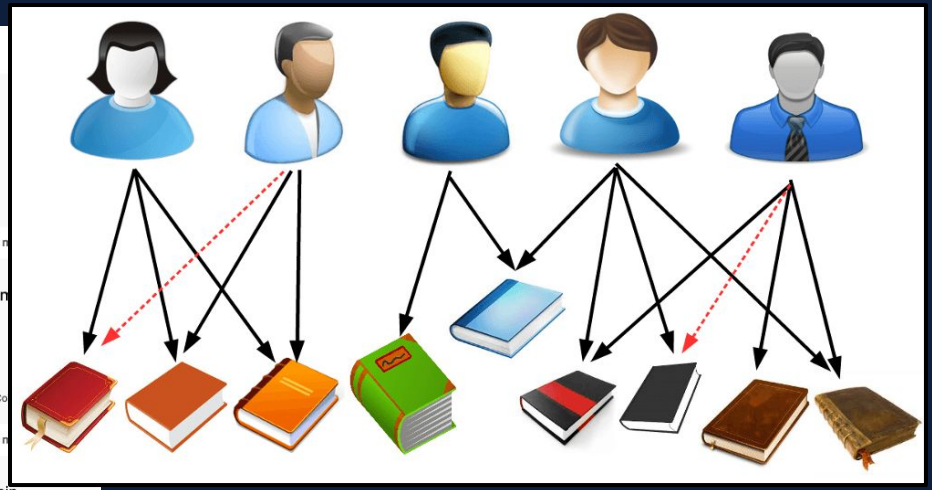
- Search spaces for CCAI applications
- Benchmark NAS on CCAI applications



Tu et al., 2022

Recommender Systems





A Worrying Analysis of Recommender Systems

Are We Really Making Much Progress? A Worrying Analysis of Recent Neural Recommendation Approaches

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ABSTRACT

Deep learning techniques have become the method of choice for researchers working on algorithmic aspects of recommender systems. With the strongly increased interest in machine learning in general, it has, as a result, become difficult to keep track of what represents the state-of-the-art at the moment, e.g., for top-n recommendation tasks. At the same time, several recent publications point out problems in today's research practice in applied machine learning, e.g., in terms of the reproducibility of the results or the choice of the baselines when proposing new models.

In this work, we report the results of a systematic analysis of algorithmic proposals for top-n recommendation tasks. Specifically, we considered 18 algorithms that were presented at top-level research conferences in the last years. Only 7 of them could be reproduced with reasonable effort. For these methods, it however turned out that 6 of them can often be outperformed with comparably simple heuristic methods, e.g., based on nearest-neighbor or graph-based techniques. The remaining one clearly outperformed the baselines but did not consistently outperform a well-tuned non-

1 INTRODUCTION

Within only a few years, deep learning techniques have started to dominate the landscape of algorithmic research in recommender systems. Novel methods were proposed for a variety of settings and algorithmic tasks, including top-n recommendation based on long-term preference profiles or for session-based recommendation scenarios [36]. Given the increased interest in machine learning in general, the corresponding number of recent research publications, and the success of deep learning techniques in other fields like vision or language processing, one could expect that substantial progress resulted from these works also in the field of recommender systems. However, indications exist in other application areas of machine learning that the achieved progress—measured in terms of accuracy improvements over existing models—is not always as strong as expected.

Lin [25], for example, discusses two recent neural approaches in the field of information retrieval that were published at top-level conferences. His analysis reveals that the new methods do *not* significantly outperform existing baseline methods when these

Family	*Method*	*Description*
Non-personalized	TopPopular	Recommends the most popular items to everyone [18]
Nearest-Neighbor	UserKNN	User-based k-nearest neighbors [58]
	ItemKNN	Item-based k-nearest neighbors [61]
Graph-based	$P^3\alpha$	A graph-based method based on random walks [16]
	$RP^3\beta$	An extension of $P^3\alpha$ [54]
Content-Based and Hybrid	ItemKNN-CBF	ItemKNN with content-based similarity [43]
	ItemKNN-CFCBF	A simple item-based hybrid CBF/CF approach [50]
	UserKNN-CBF	UserKNN with content-based similarity
	UserKNN-CFCBF	A simple user-based hybrid CBF/CF approach
Non-Neural Machine Learning	iALS	Matrix factorization for implicit feedback data [33]
	pureSVD	A basic matrix factorization method [18]
	SLIM	A scalable linear model [36, 52]
	$EASE^R$	A recent linear model, similar to auto-encoders [63]

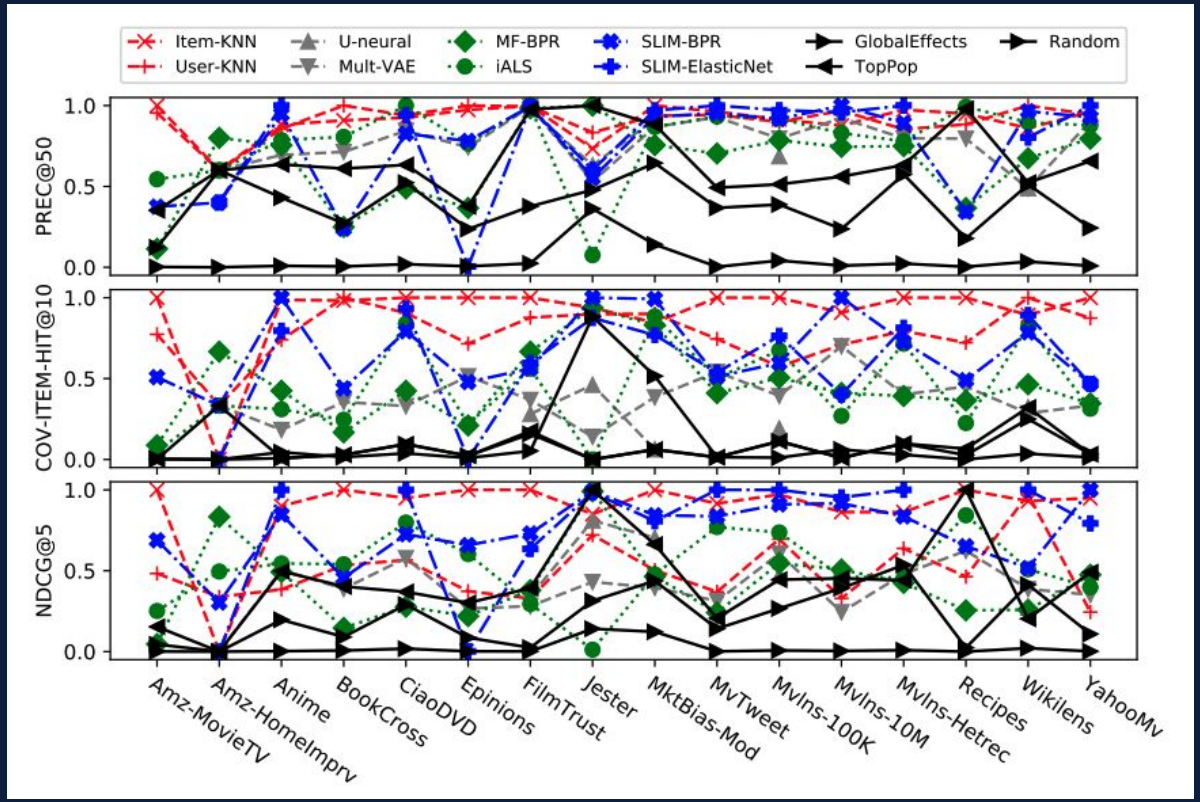
Meta-Learning for Recommender Systems

- 24 Algorithms, up to 100 hyperparameters, 85 datasets, 315 metrics

Rank	Item-KNN	P3alpha	SLIM-BPR	EASE-R	RP3beta	SVD	SLIM-ElasticNet	iALS	NMF	User-KNN	MF-Funk	TopPop	MF-Asy	MF-BPR	Mult-VAE	U-neural	GlobalEffects	CoClustering	Random	SlopeOne
Min.	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	2	1	9	7
Max.	14	18	14	18	17	16	17	19	14	17	18	19	16	17	20	20	20	19	20	20
Mean	2.3	4.2	4.7	5.3	6	6	7	7	7.1	7.6	9.4	10.4	10.7	11.2	11.7	12.3	13.3	14.9	16.2	16.7

RecZilla, 2022

Meta-Learning for Recommender Systems

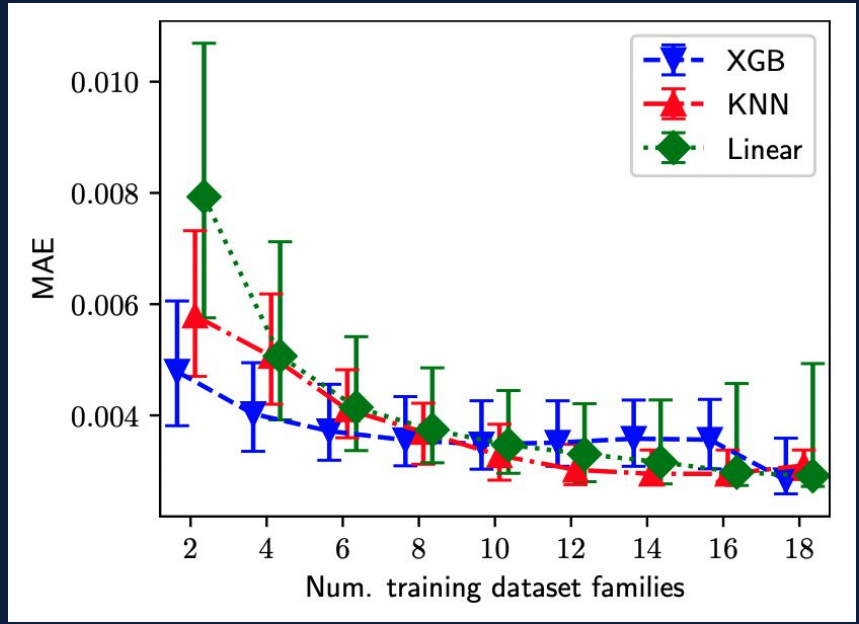


RecZilla, 2022

RECZILLA

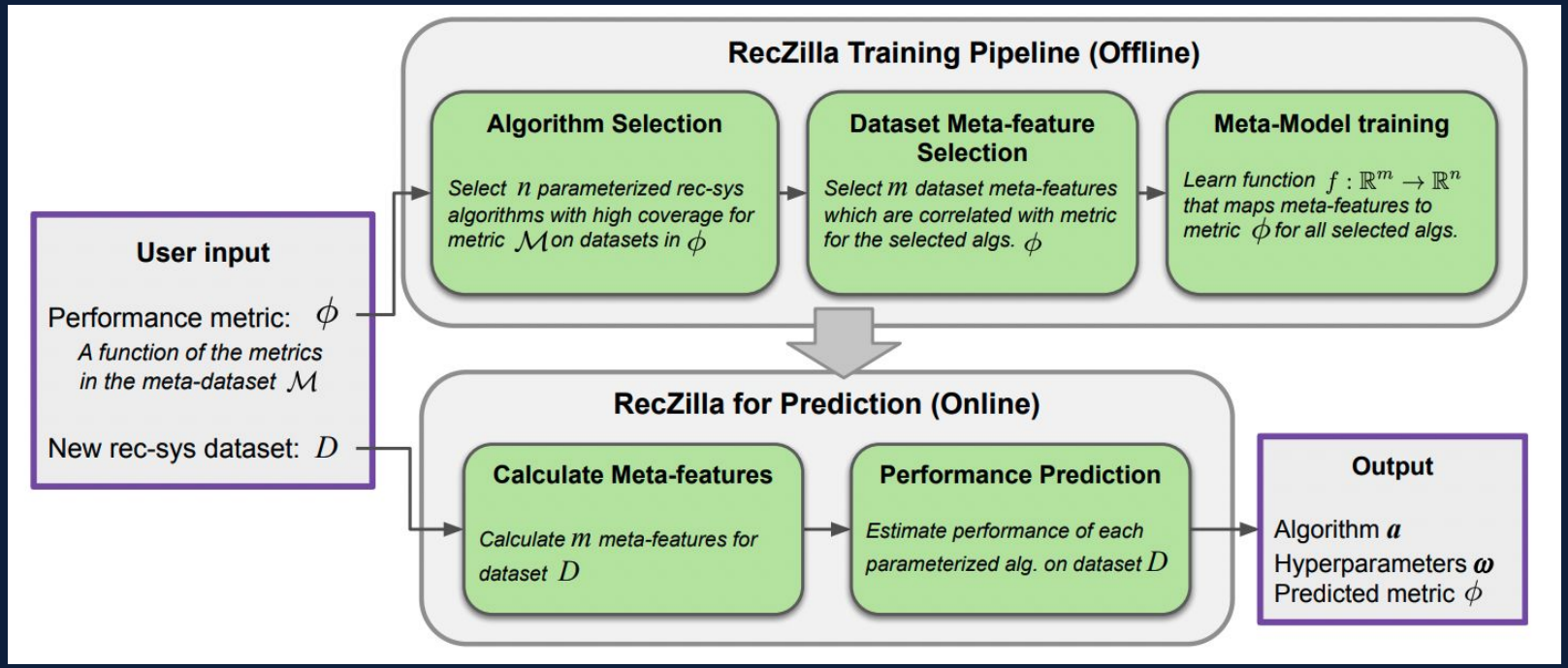
Dataset meta-features

- User distribution
- Item distribution
- Interaction distribution
- Landmarkers



RecZilla, 2022

RECZILLA



RecZilla, 2022

Thanks! Questions?

colin@abacus.ai

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