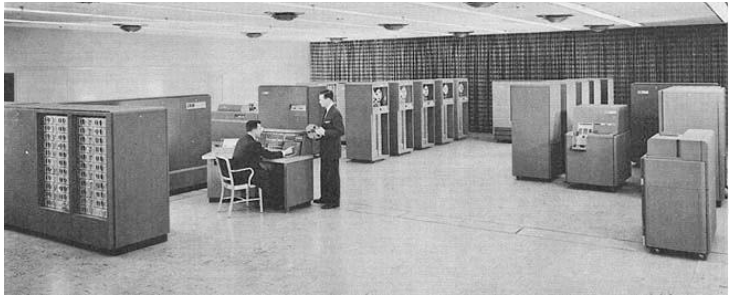
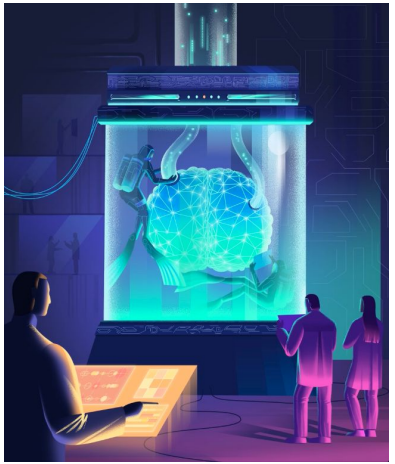
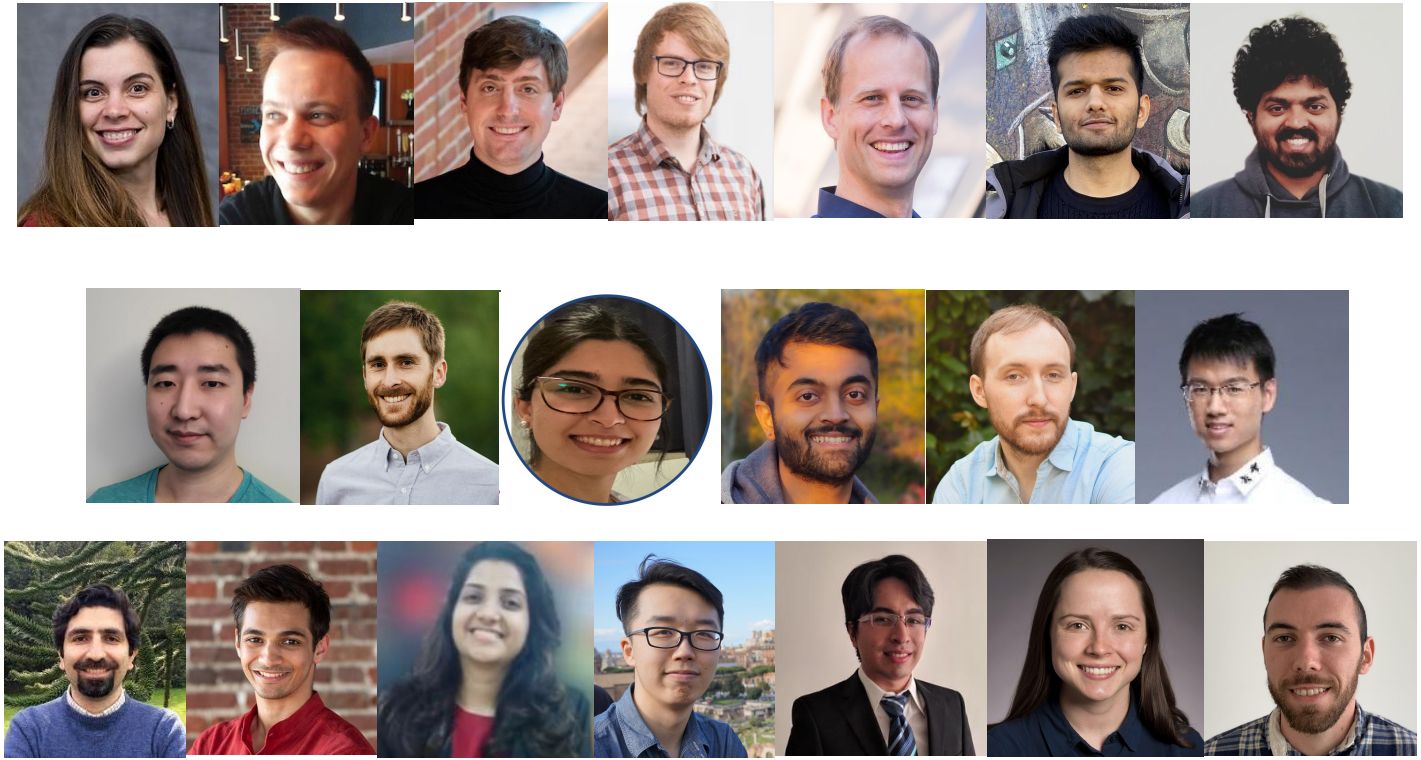
Neural Architecture Search: The Next Frontier





Colin White
colin@abacus.ai
https://crwhite.ml/



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

NVIDIA

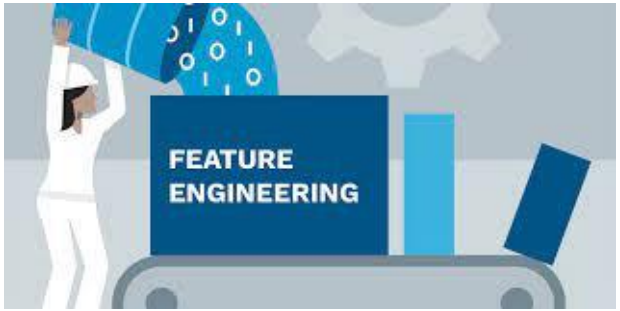
ABACUS.AI

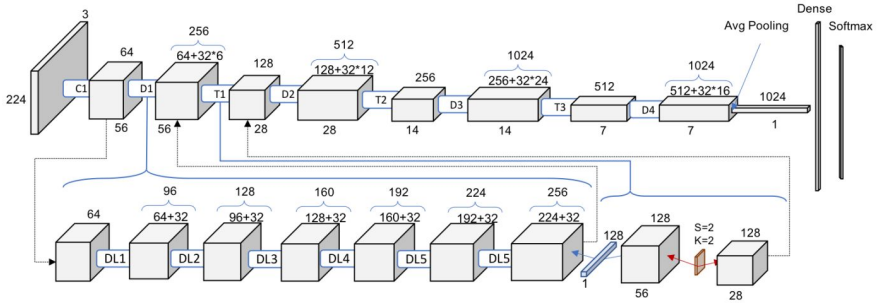
1950s

2012

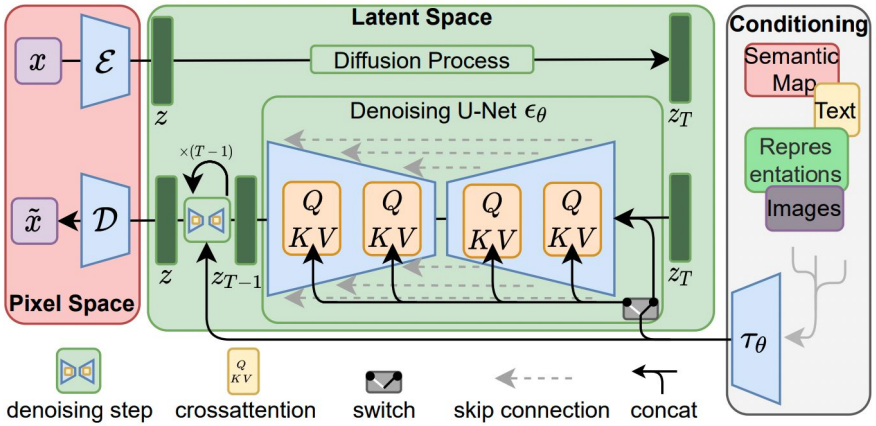
2017

2023

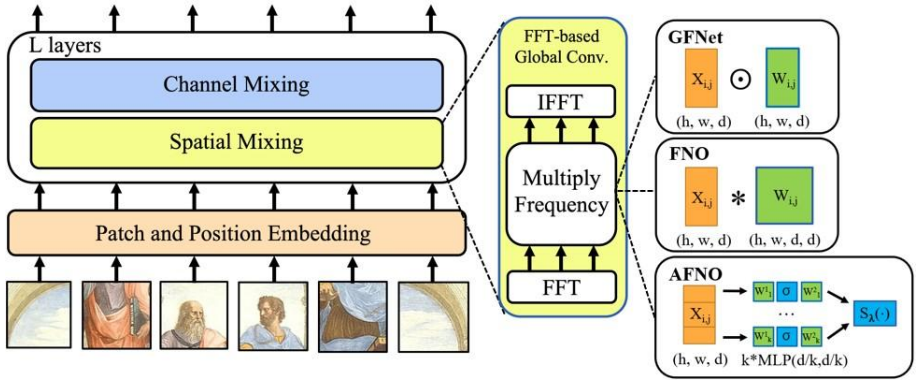




DenseNet (2016)

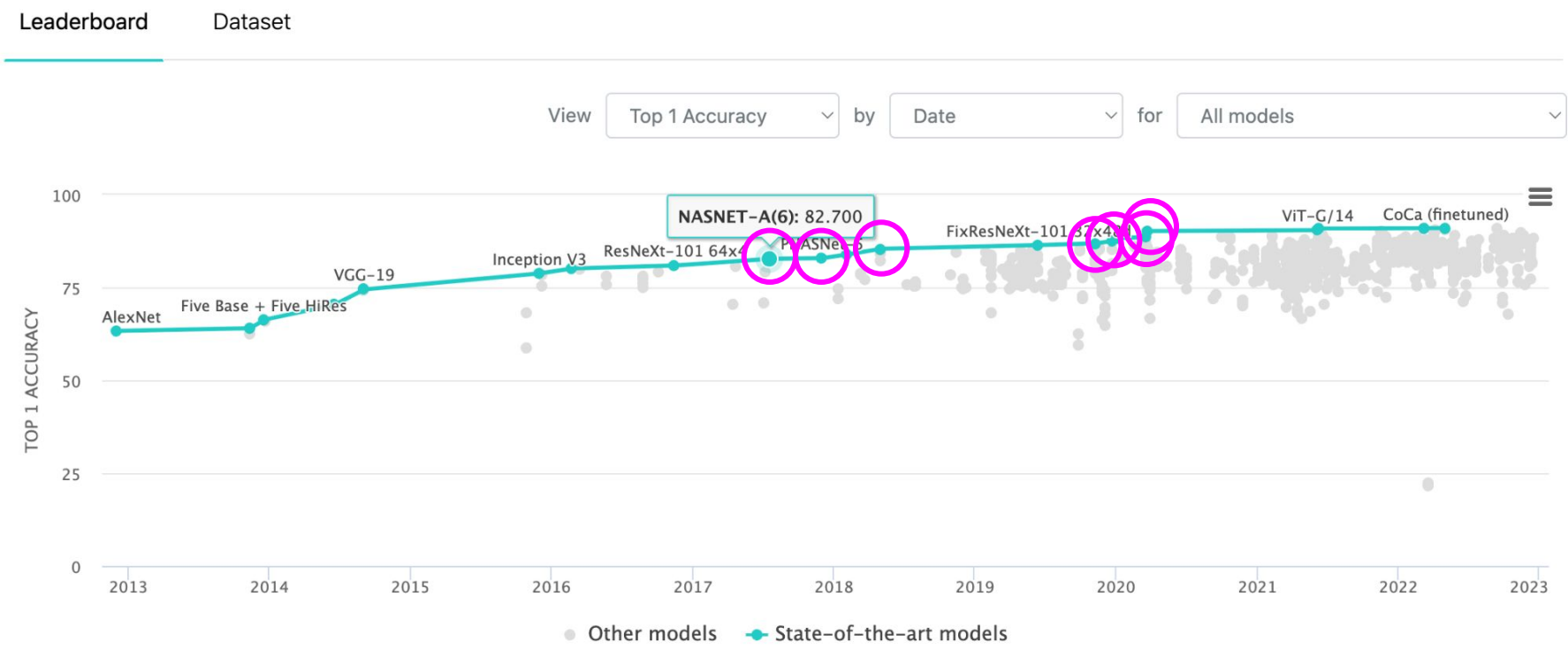


Stable Diffusion (2022)



AFNO (2022)

State of the Art on ImageNet



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

NVIDIA

ABACUS.AI

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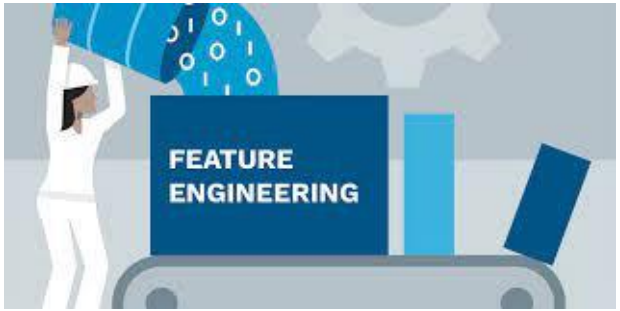
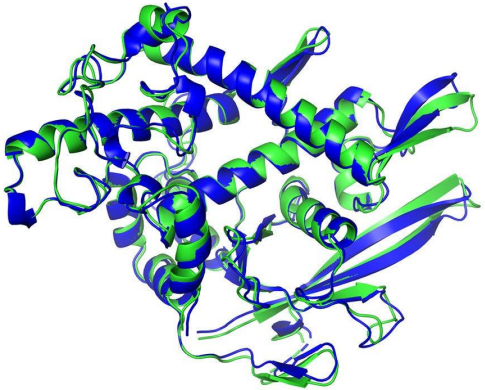
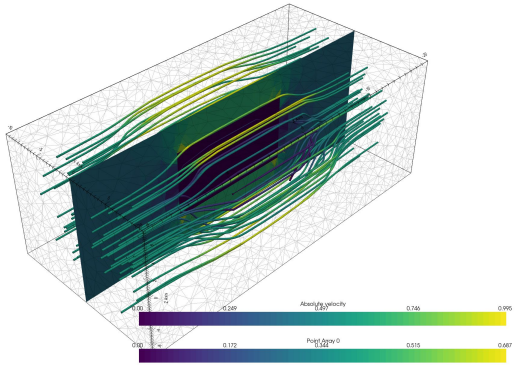
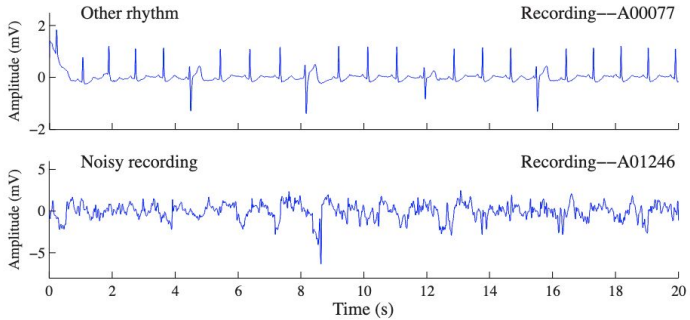
2023



Diverse Tasks



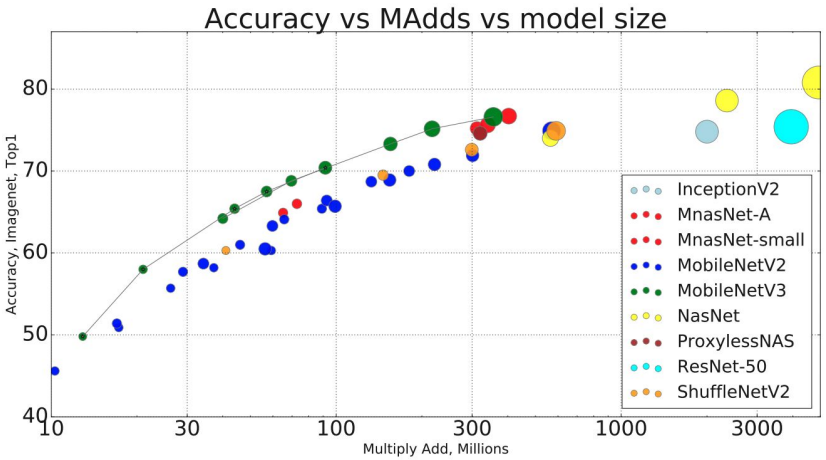




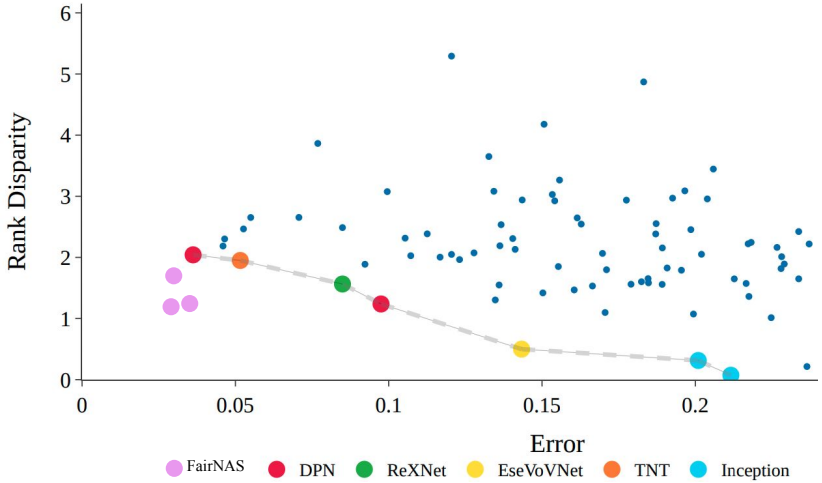
TRKSST (2022)

TRPNJSRTNW (2022)

Multi-Objective



HSCCCTWZPVLA (2019)



SDDWHG (2022)

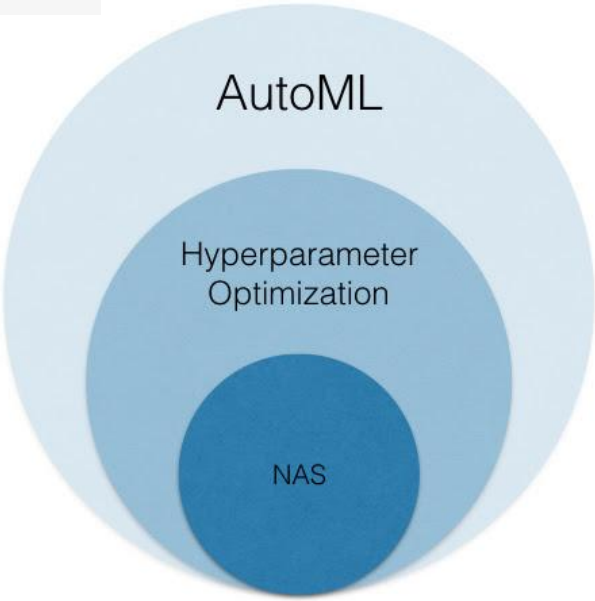
What is neural architecture search?

Neural architecture search (NAS) is a technique for automatically finding the best architecture for a neural network for a particular task. It involves using a search algorithm to explore the space of possible network architectures, and selecting the one that performs the best on a given dataset.

Given a search space *A*,

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

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



Automate the design of **high-performing** models using **theoretical analyses**, **algorithm design**, and large-scale **empirical analyses**.

Neural architecture search

WNNS (NeurIPS 2020)
WNS (AAAI 2021)
WNS (UAI 2021)
Y*W*SH (NeurIPS 2021)
WZRLH (NeurIPS 2021)
M*W*ZKZMSYH (ICLR 2022)
WKTSBD ICLR-Blog (2022)
K*W*T*Z*SH (NeurIPS 2022)
PWJNIR (arXiv 2022)
WSSREZDH (preprint 2023)

Hyperparameter optimization

BNVW (COLT 2017)
BDW (NeurIPS 2018)
MKVDW (NeurIPS 2022)

Bias & explainability

SWG (NeurIPS 2020)
LKWN (NeurIPS 2021)
SDDWHG (arXiv 2022)

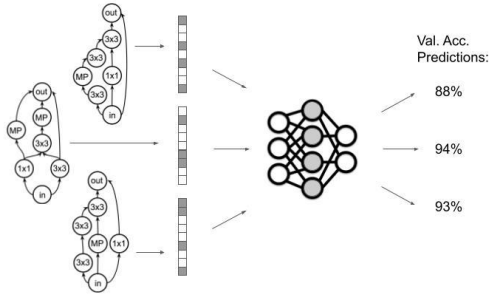
Enabling good scientific practices

Outline

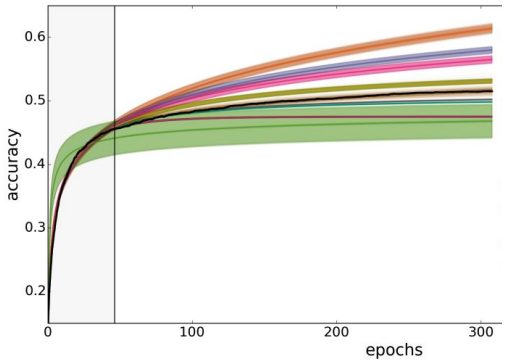
- Introduction
- **NAS**
  - **Algorithm design**
  - **Mitigating bias**
- HPO: theoretical results
- Future directions

Performance Prediction

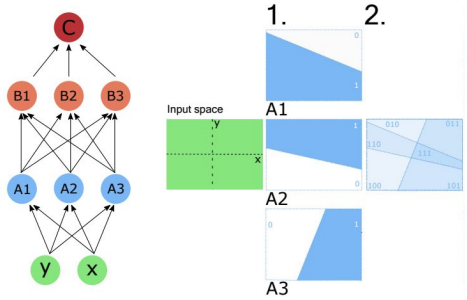
Predict the (relative) accuracy of an architecture, without fully training it



Model-based



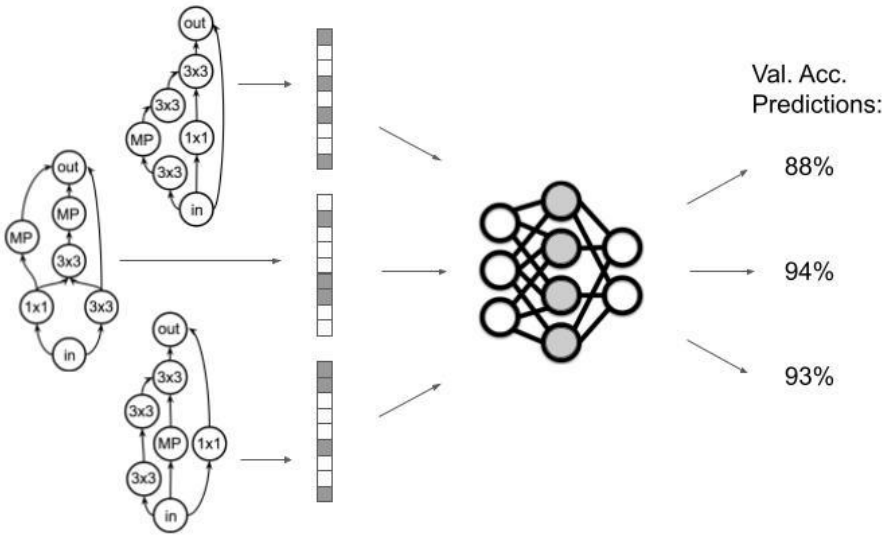
Learning curve extrapolation



Zero-cost proxies

Model-Based Predictors

Train a surrogate model



- Gaussian processes
  - KNSPX (2018)
  - JSH (2018)
- Boosted trees
  - LTWQCL (2020)
  - ZSZLKH (2020)
- GNNs
  - SPXLKZ (2019)
  - WLLCBK (2019)
- Specialized encodings
  - WNS (2019)
  - NZZWY (2020)

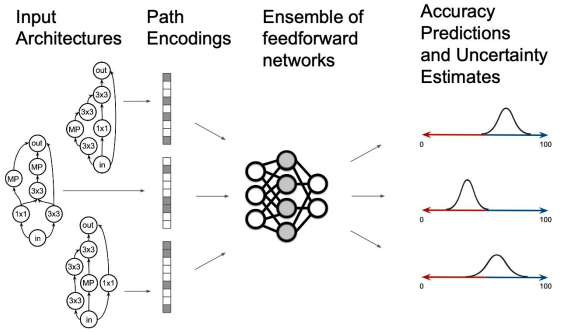
"BO + Neural Predictor" Components

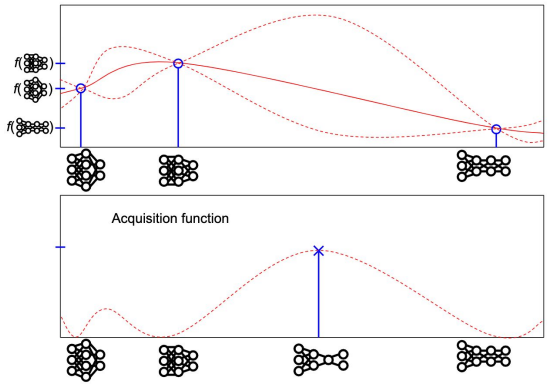
Algorithm 1 BANANAS

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.

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





WNS (2019), SPXLKZ (2019), MCY (2019)

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

WNS (AAAI 2021)

BANANAS

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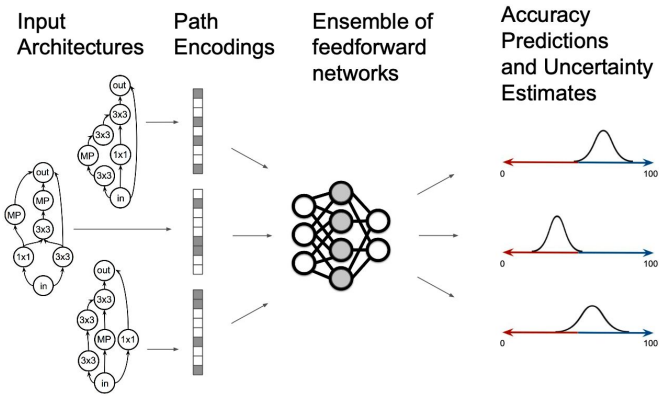
WNS (AAAI 2021)



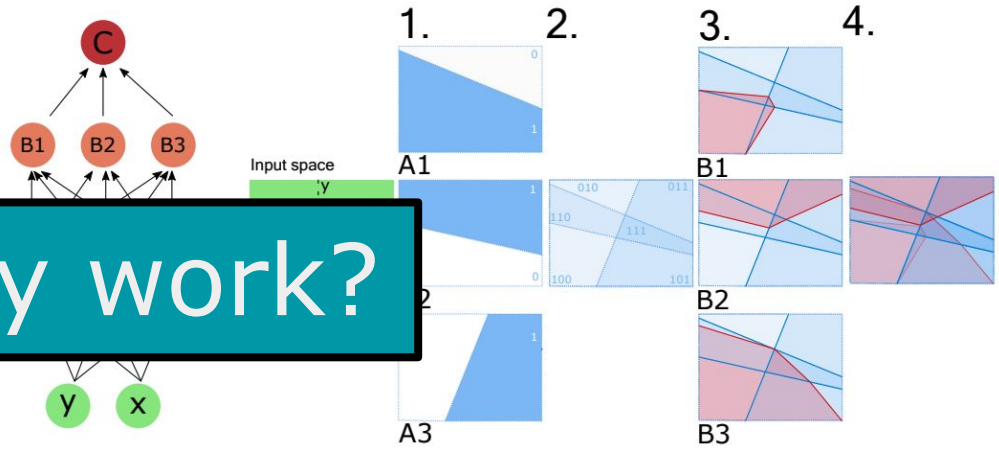
Path encoding, ensemble

Small mutations

Independent Thompson Sampling

Zero-cost proxies

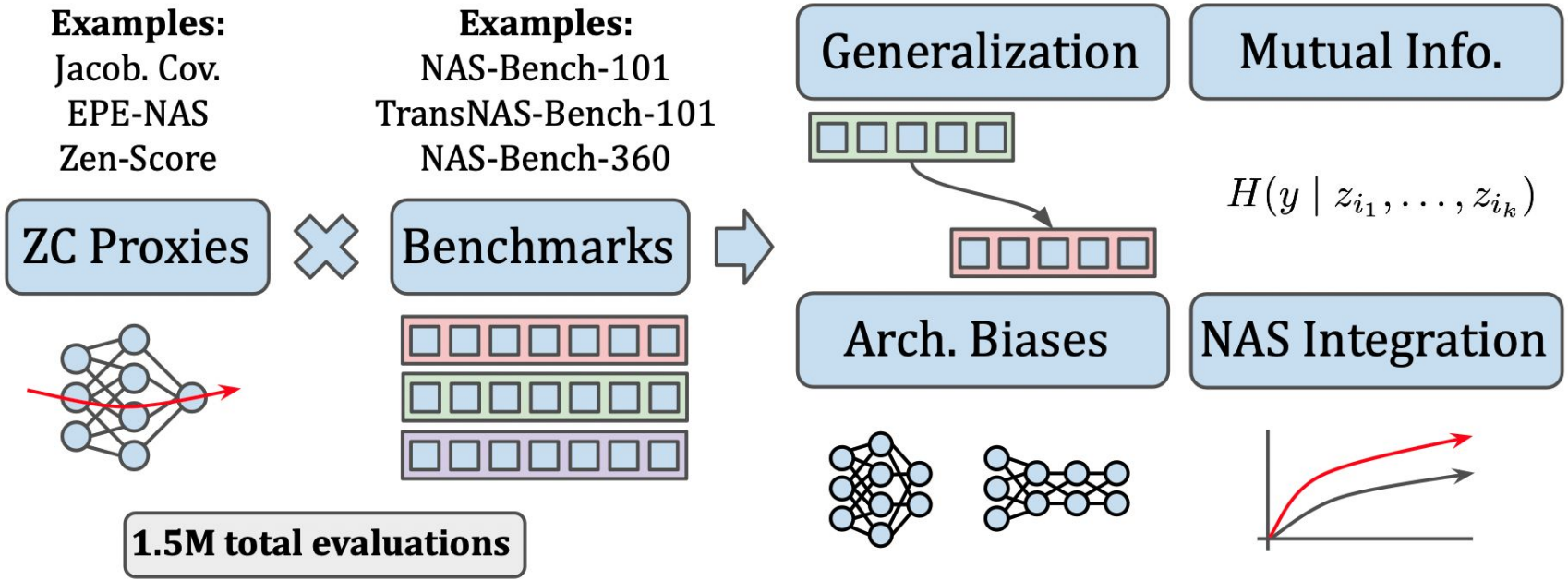
epe-nas [21]	Jacobian
fisher [42]	Pruning-at-init
flops [25]	Baseline
grad-norm [1]	Pruning-at-init
grasp [43]	Pruning-at-init
l2-norm [1]	B
jacov [23]	Ja
nwot [23]	Ja
params [25]	Baseline
plain [1]	Baseline
snip [14]	Pruning-at-init
synflow [39]	Pruning-at-init
zen-score [16]	Piece. Lin.



Do they work?

MTSC (2020)

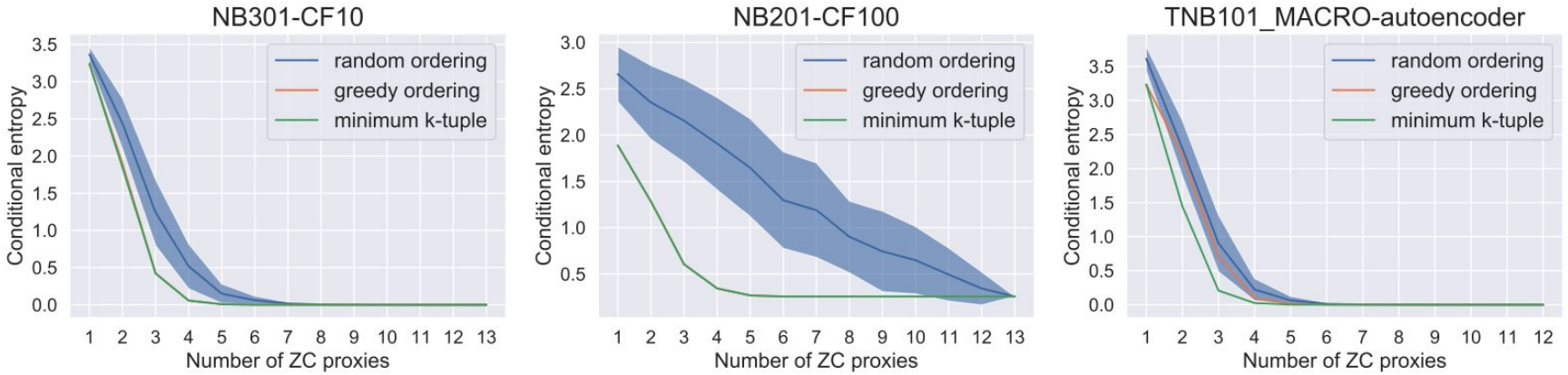
Compute an estimate in 5 seconds



WKTSBD (ICLR-Blog 2022)

K*W*Z*T*SH (NeurIPS 2022)

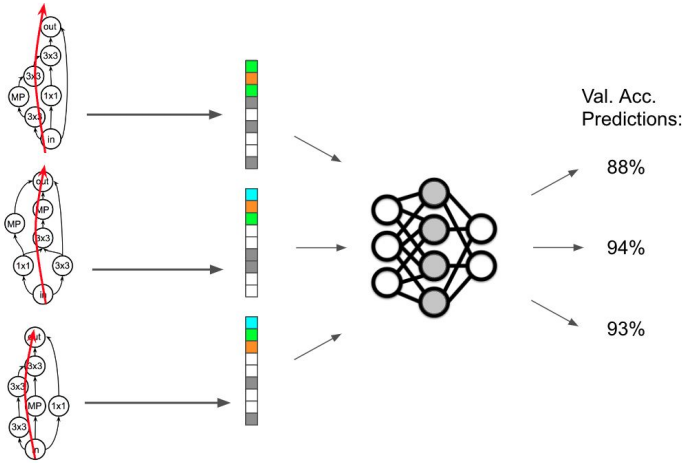
Complementary Information



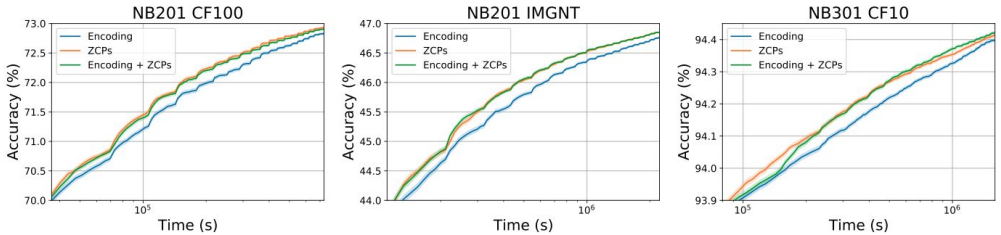
Conditional entropy $H(y \mid z_{i_1}, \ldots, z_{i_k})$ vs. k

K*W*Z*T*SH (NeurIPS 2022)

NAS integration



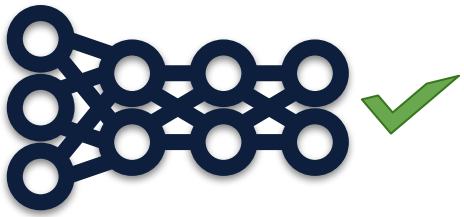
Features Benchmark	Encoding	ZC	Both	% Improvement (ZC)	% Improvement (Both)
NB101-CF10	0.546	0.708	0.718	29.67	31.50
NB201-CF10	0.622	0.905	0.906	45.50	45.66
NB201-CF100	0.640	0.907	0.908	41.71	41.87
NB201-IMGNT	0.683	0.879	0.883	28.70	29.28
NB301-CF10	0.314	0.405	0.465	28.98	48.09
TNB101_MACRO-AUTOENC	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

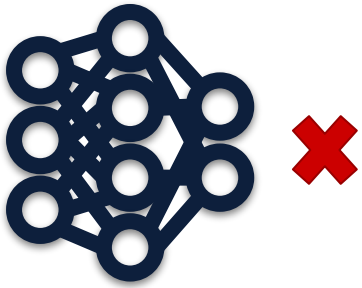


K*W*Z*T*SH (NeurIPS 2022)

Removing Biases

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



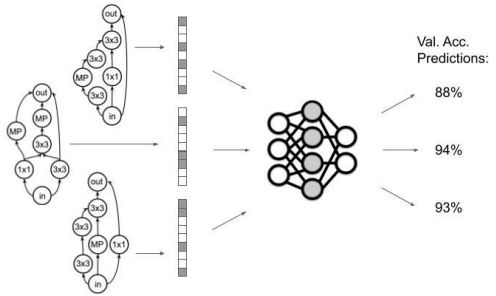


ZC proxy	dataset	bias metric	original bias	original perf.	new bias	new perf.	strategy
l2-norm	NB201-CF10	conv:pool	0.87	0.42	0.00	0.10	minimize
					0.37	0.11	equalize
					0.70	0.44	performance
nwot	NB301-CF10	conv:pool	0.78	0.49	0.00	0.03	minimize
					0.29	0.14	equalize
					0.78	0.49	performance
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

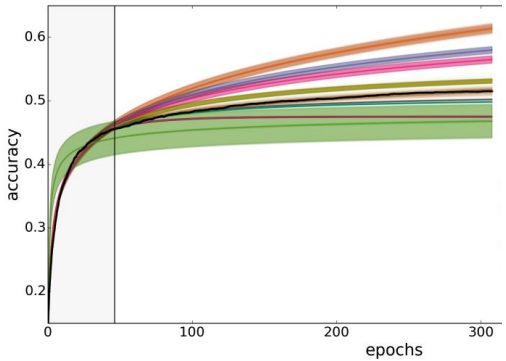
K*W*Z*T*SH (NeurIPS 2022)

Performance Prediction

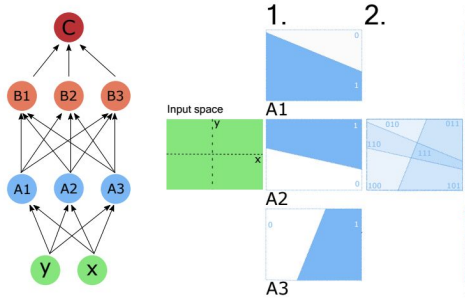
Predict the (relative) accuracy of an architecture, without fully training it



Model-based



Learning curve extrapolation



Zero-cost proxies

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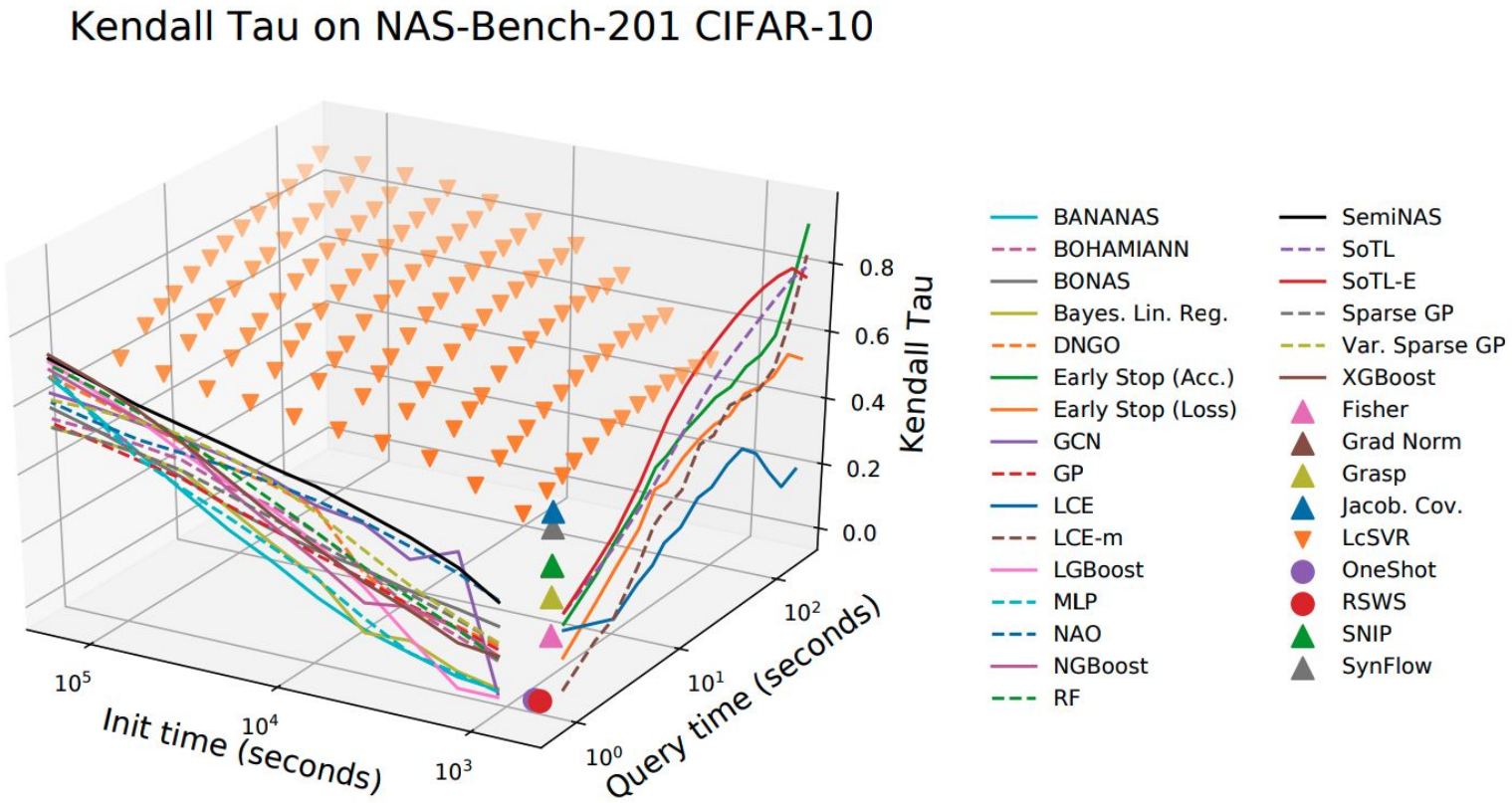
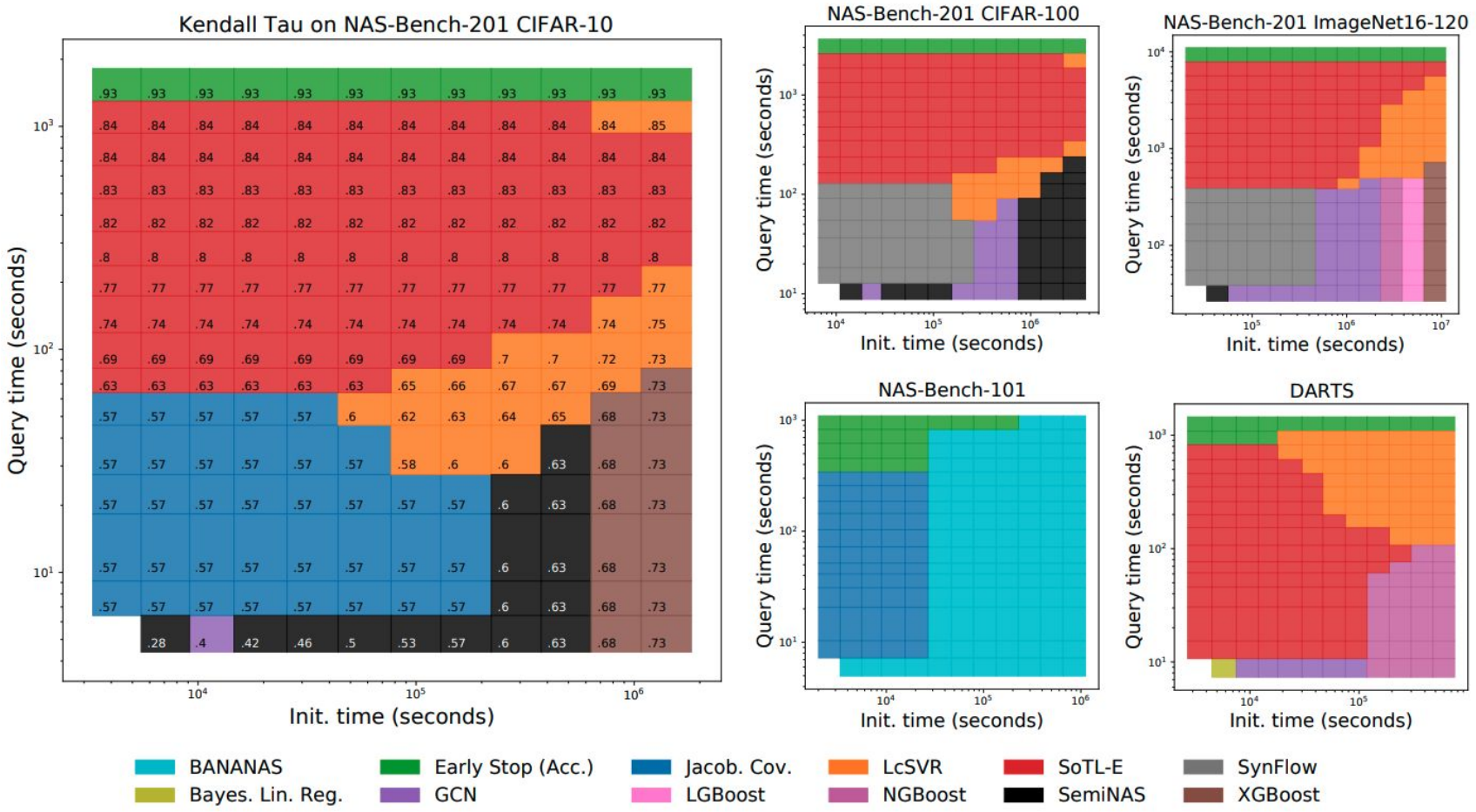


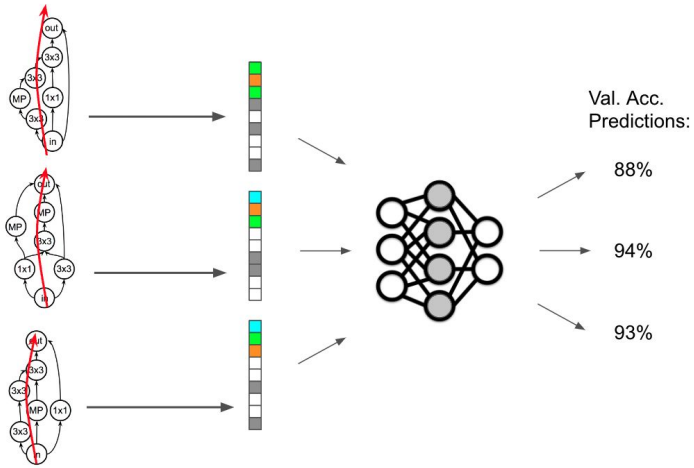
WZRLH (NeurIPS 2021)

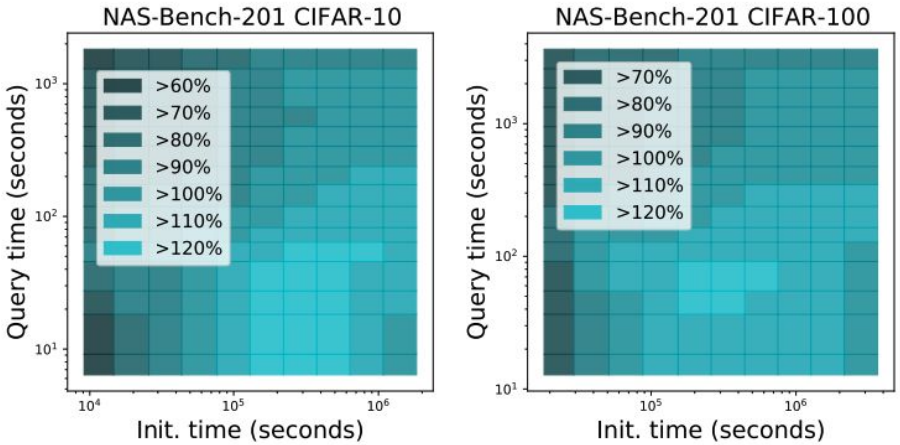


WZRLH (NeurIPS 2021)

The Omnipotent Predictor

Combine best predictors from each family





WZRLH (NeurIPS 2021)

How do we set up
neural architecture search
for a new application?

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

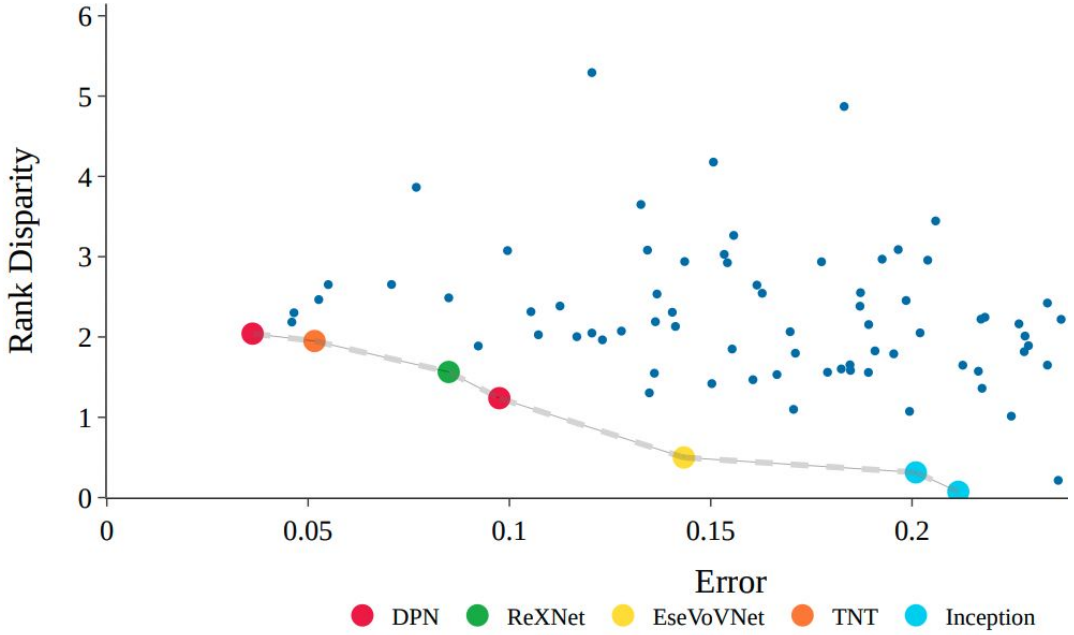
https://www.nist.gov/news-events/news/2019/12/nist-study-evaluates-effects-race-age-sex-face-recognition-software

Architectures

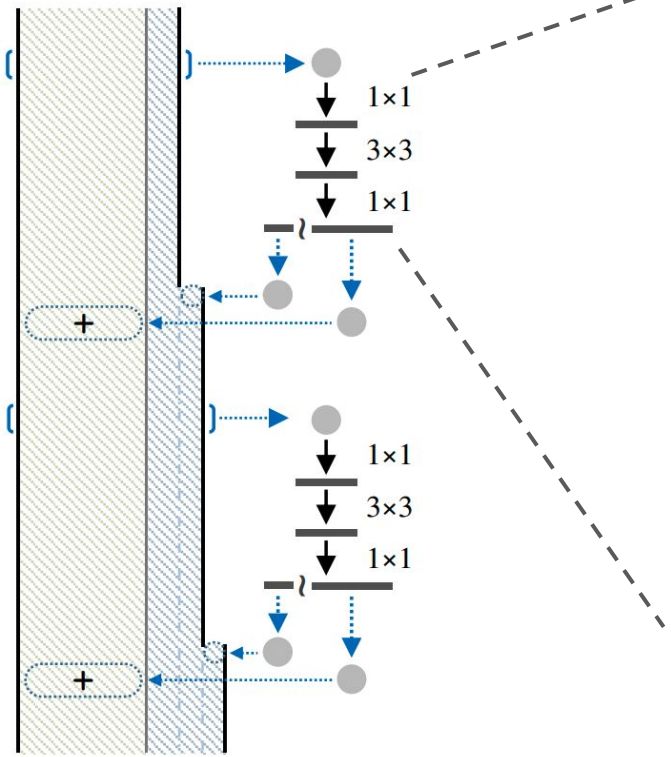
Examples:
Inception
ViTransformer
VovNet
MobileNetV3
Dual Path Net

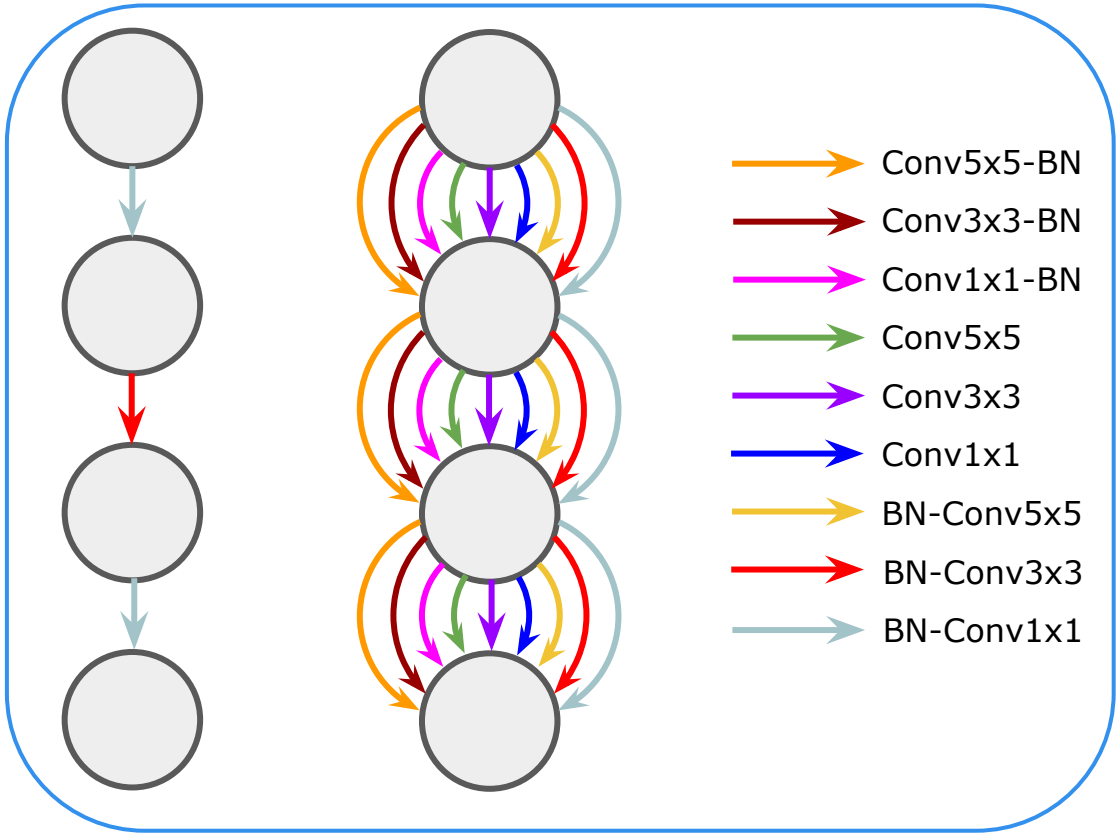
Hyperparams

Examples:
MagFace (head)
ArcFace (head)
CosFace (head)
Optimizer
Learning Rate



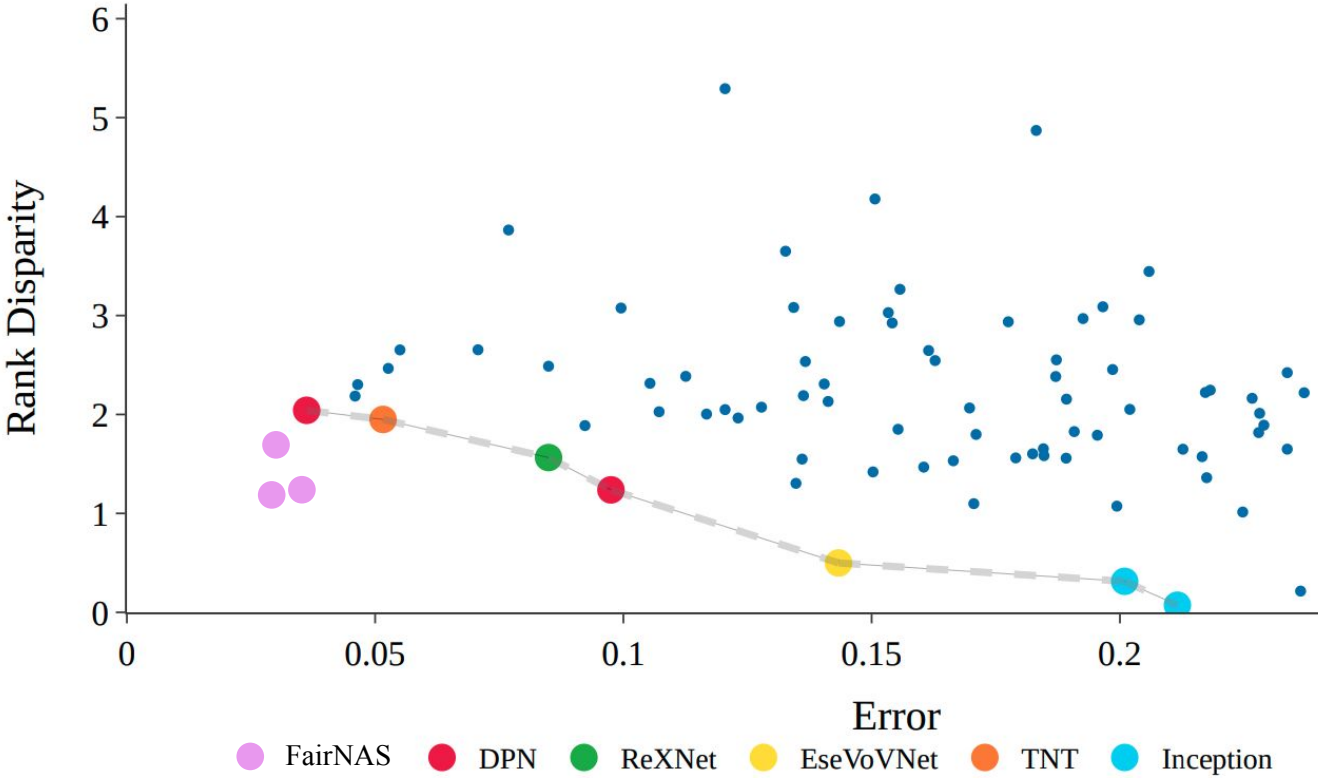
SDDWHG (arXiv 2022)





DPN (2018)

SDDWHG (arXiv 2022)



SDDWHG (arXiv 2022)

Outline

- Introduction
- NAS: algorithm design
- **HPO: theoretical results**
- Future directions

Data-Driven Algorithm Design

Optimization for **one** dataset

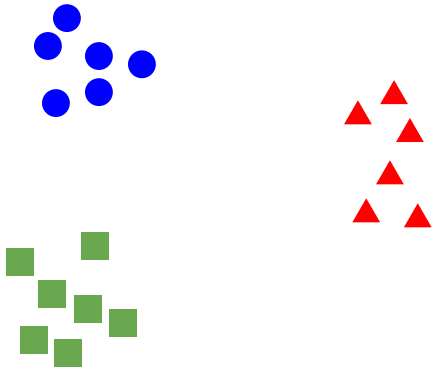
Optimization for a **distribution** of datasets

Supervised learning

Unsupervised learning (clustering)

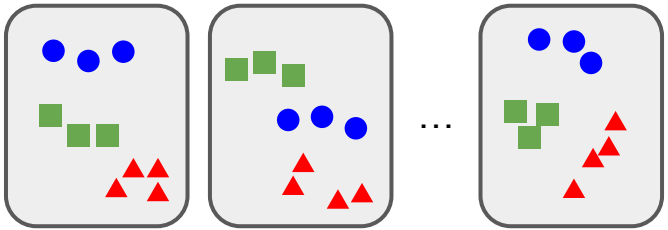
Clustering

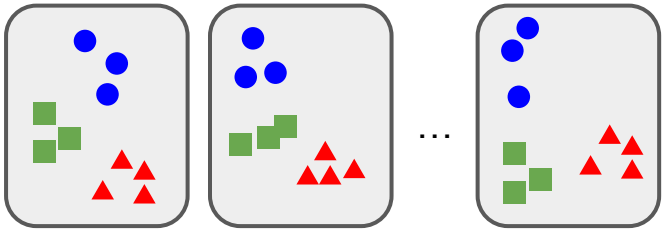
Input: dataset, *k*



- Find *k* clusters
- Minimize distance to ground-truth clustering

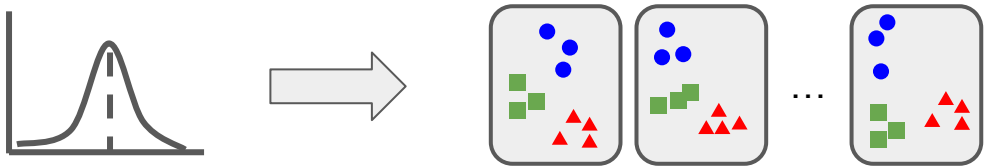
Data-Driven Algorithm Design





Data-Driven Algorithm Design

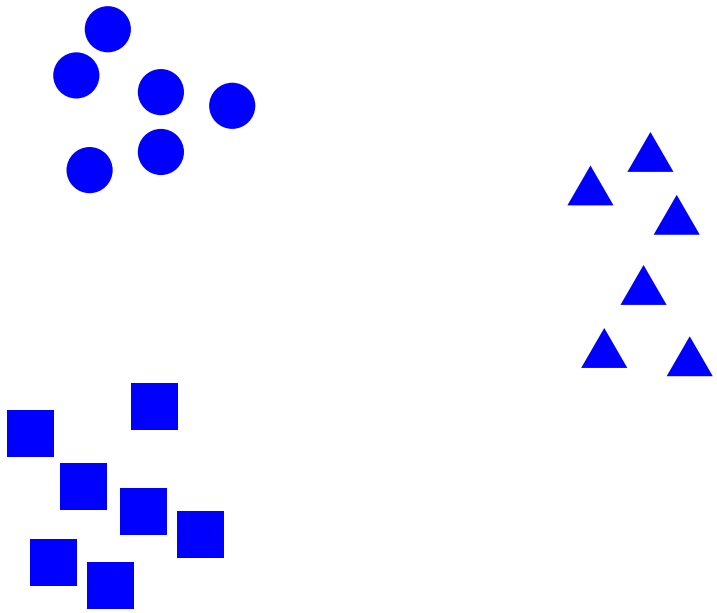
- Fix a parameterized clustering algorithm
- Receive training set of “typical” clustering instances



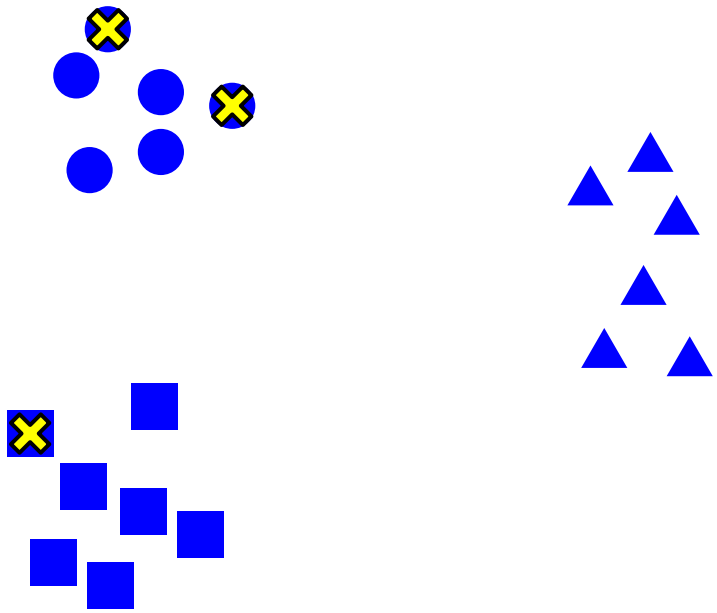
- Find hyperparameters with good average performance

How to find high-performing hyperparameters?
Will these hyperparameters have strong future performance?

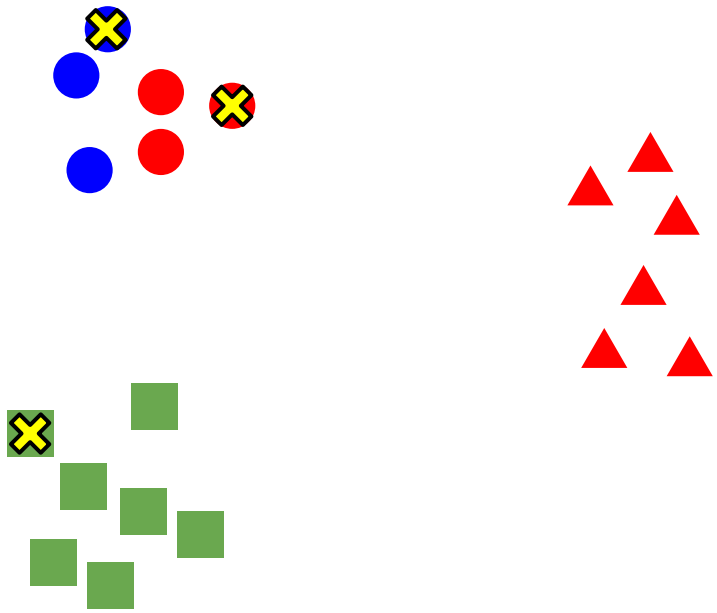
k-means



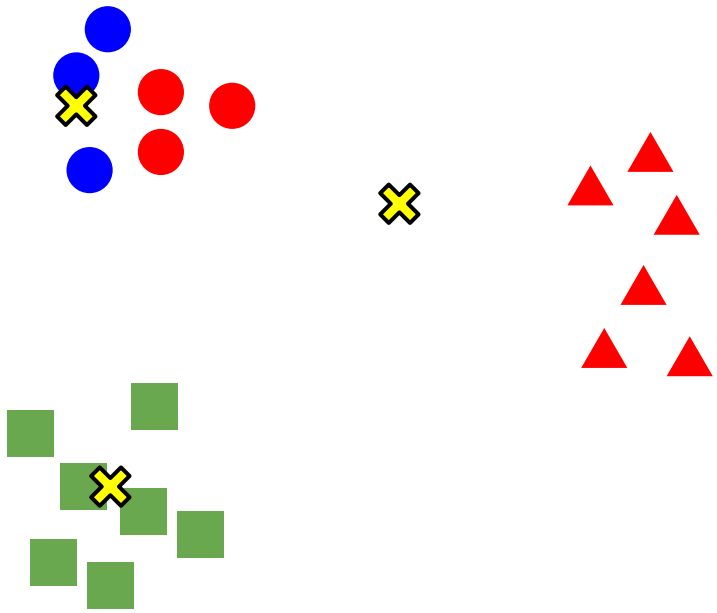
k-means



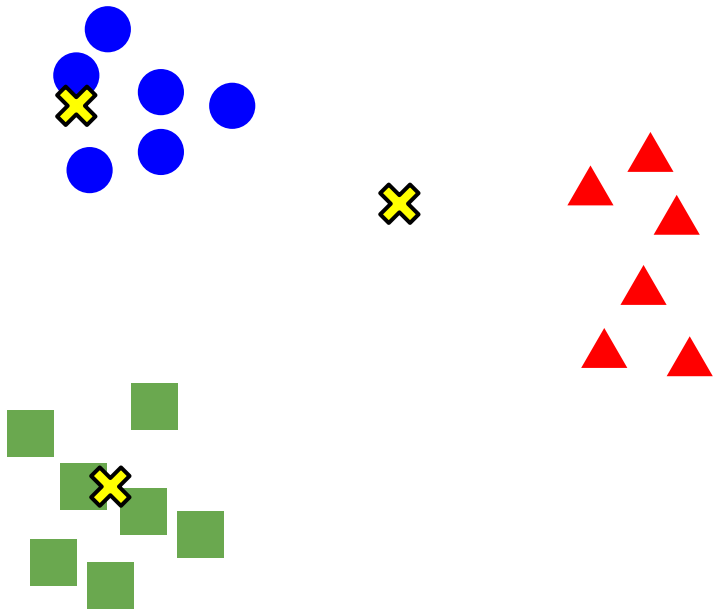
k-means



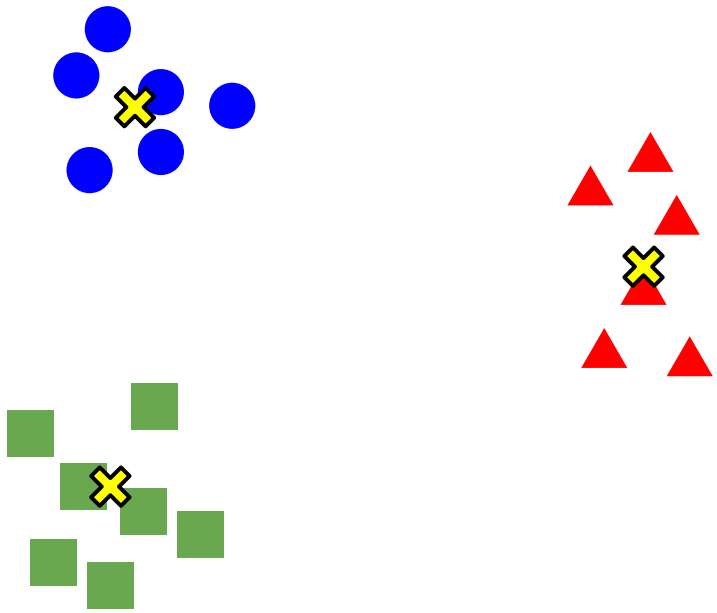
k-means



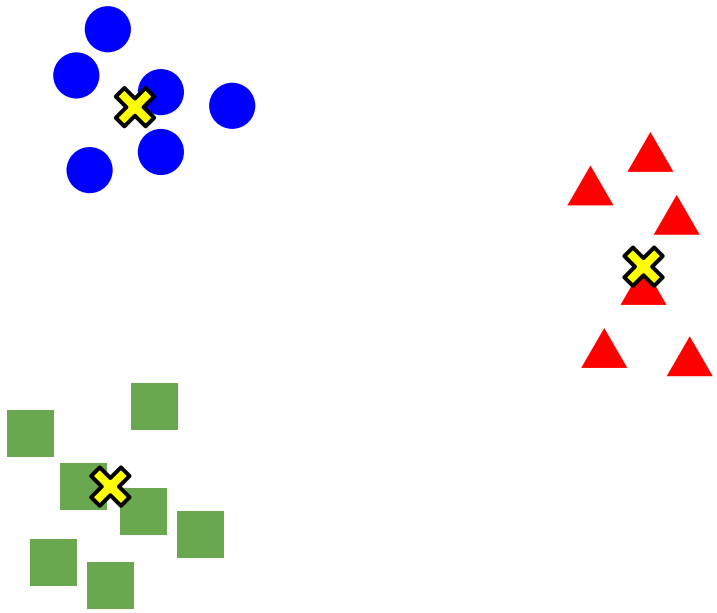
k-means



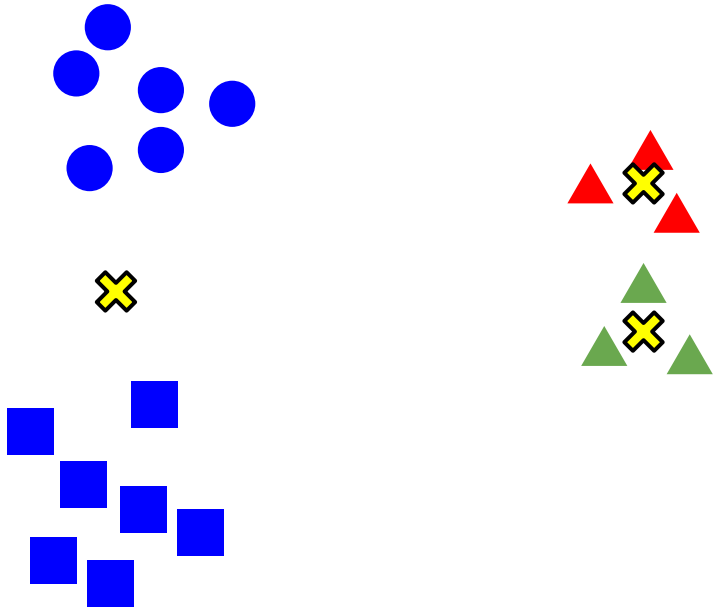
k-means



k-means

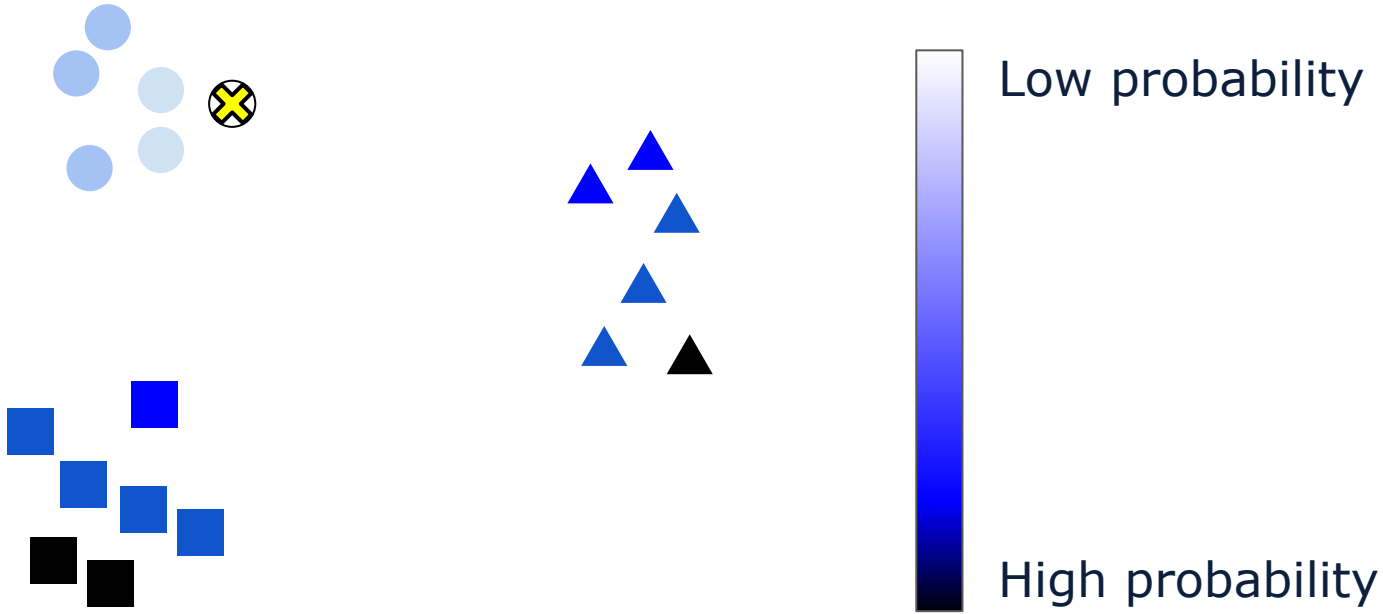


Initial centers are important!



k-means++

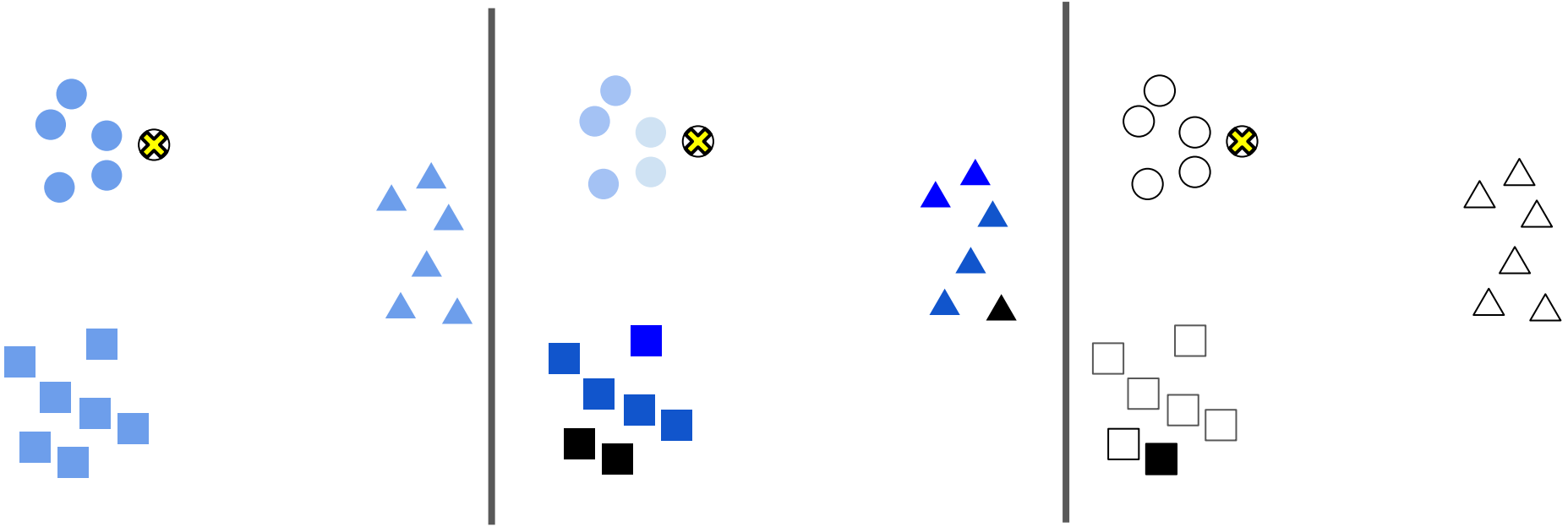
d^2 sampling



A new family of clustering algorithms

d^{α} sampling β-local search

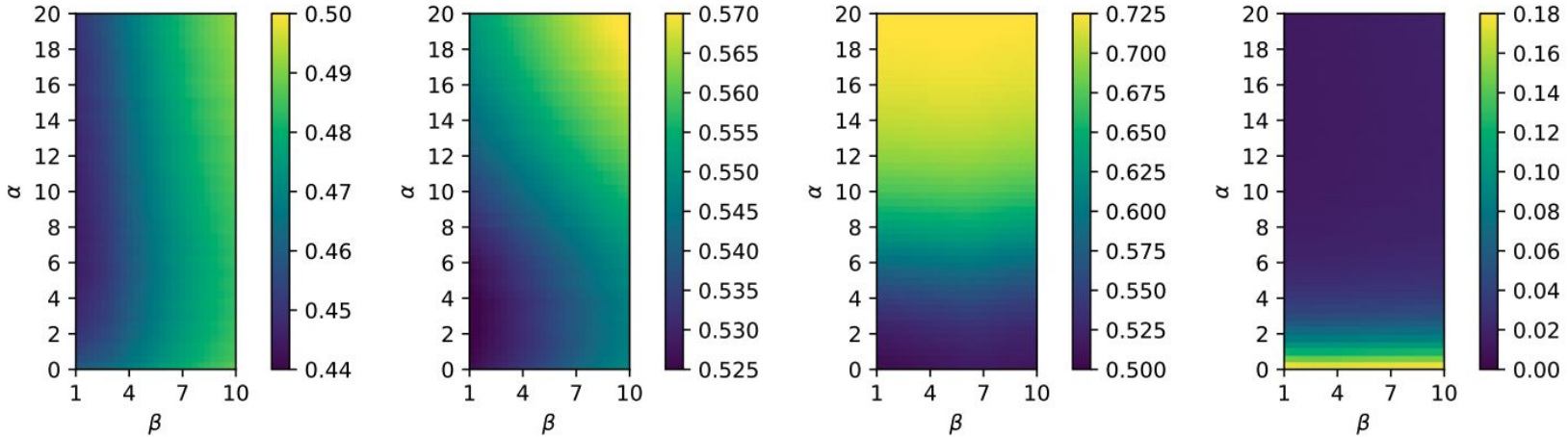
$\alpha = 0$ $\alpha = 2$ $\alpha = \infty$



BDW (NeurIPS 2018)

A new family of clustering algorithms

d^{α} sampling β-local search



(a) MNIST (b) CIFAR-10 (c) CNAE-9 (d) Gaussian Grid

BDW (NeurIPS 2018)

Theorem: Given $\tilde{o}\left(\frac{k \log n}{\epsilon^2}\right)$ sampled clustering instances,
with high probability for all α, β,
|**Avg** performance over training set - **expected** performance| < ε.

Key intuition:

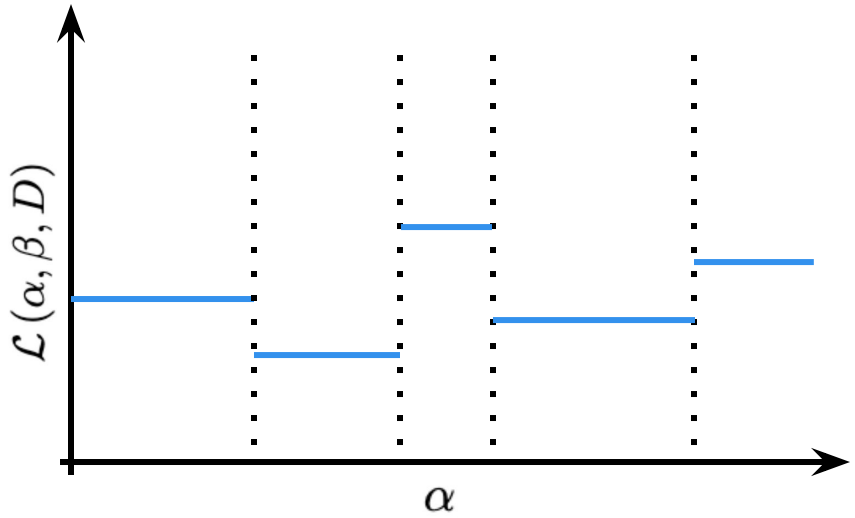
A set of hyperparameters with high performance **on the training set**, also achieves high performance **in the future**

BDW (NeurIPS 2018)

Theorem: Given $\tilde{o}\left(\frac{k \log n}{\epsilon^2}\right)$ sampled clustering instances,
with high probability for all α, β,
|**Avg** performance over training set - **expected** performance| < ε.

Key insight:

Bound the expected number
of **discontinuities** of $\mathcal{L}(\alpha, \beta, D)$
as a function of α, β

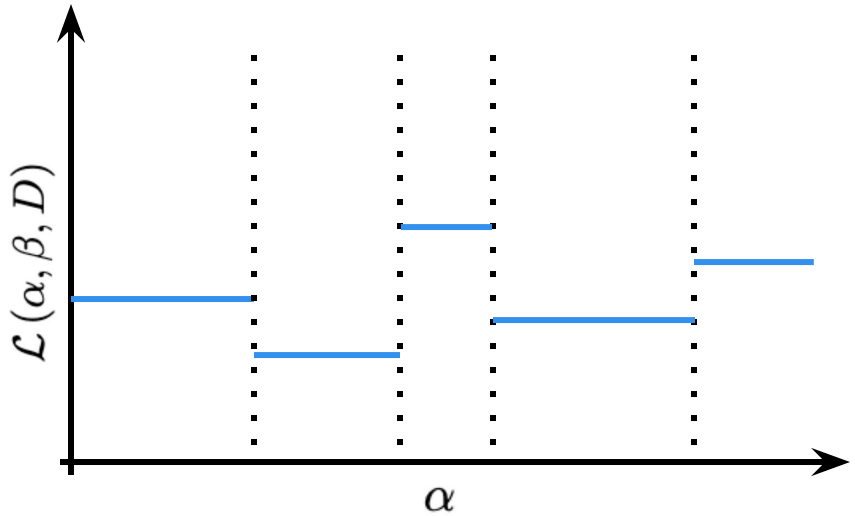


BDW (NeurIPS 2018)

Theorem: Given $\tilde{O}\left(\frac{k \log n}{\epsilon^2}\right)$ sampled clustering instances,
with high probability for all α, β,
|**Avg** performance over training set - **expected** performance| < ε.

Efficient algorithm:

Solve for the **discontinuities**



BDW (NeurIPS 2018)

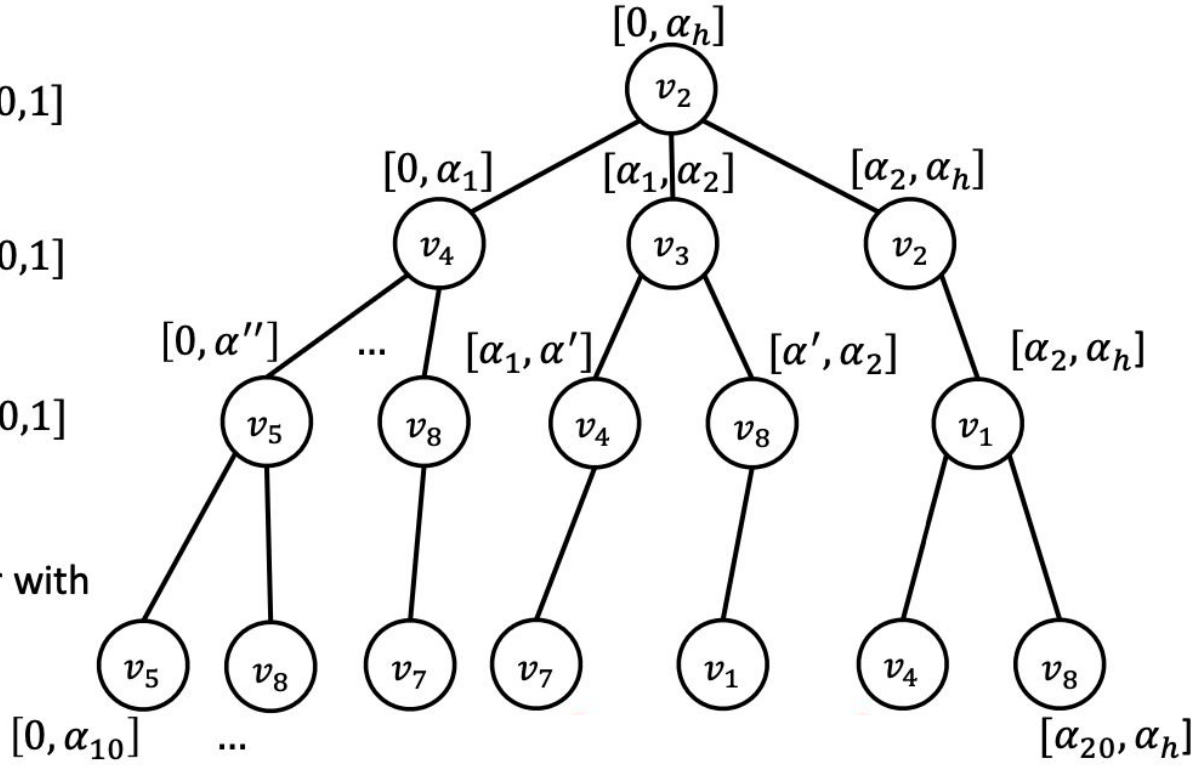
Execution Tree

Draw $z_1 \in [0,1]$

Draw $z_2 \in [0,1]$

Draw $z_3 \in [0,1]$

Full partition of $[0, \alpha_h]$ together with set of centers



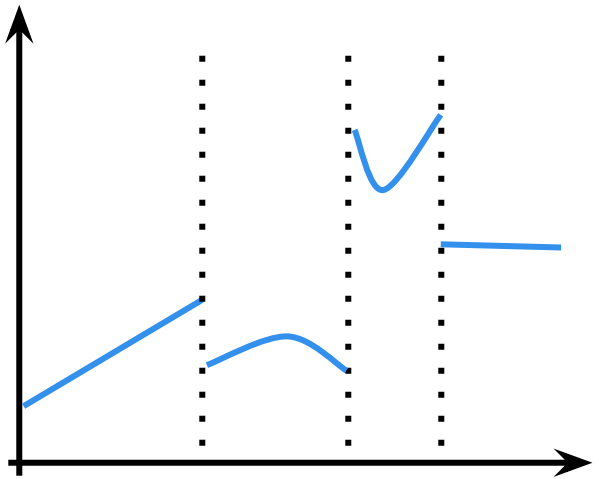
Subsequent Work

Generalizations

- Piecewise polynomial (BDDKSV, 2019)
- Approximately piecewise polynomial (BSV, 2020)

Beyond clustering

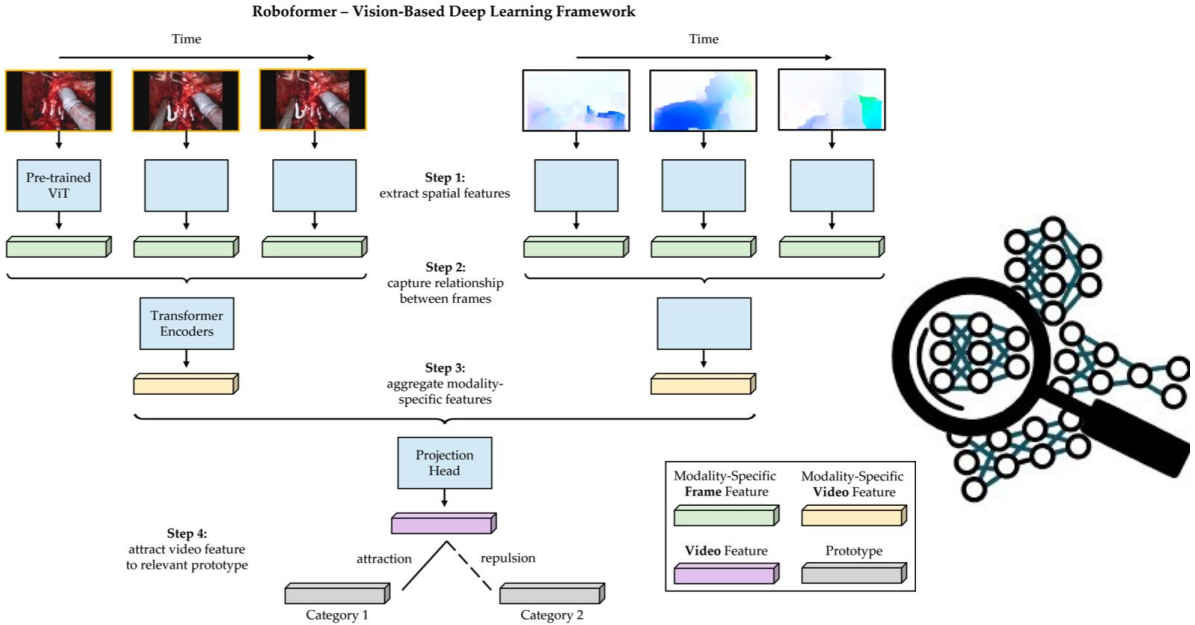
- Integer Programming (BDV, 2018)
- ElasticNet (BKST, 2022)



Outline

- Introduction
- NAS: algorithm design
- HPO: theoretical results
- **Future directions**
  - **Surgical AI**
  - **Climate sciences**

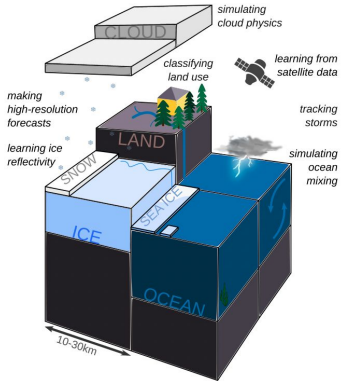
Tackling Surgical AI with **AutoML**

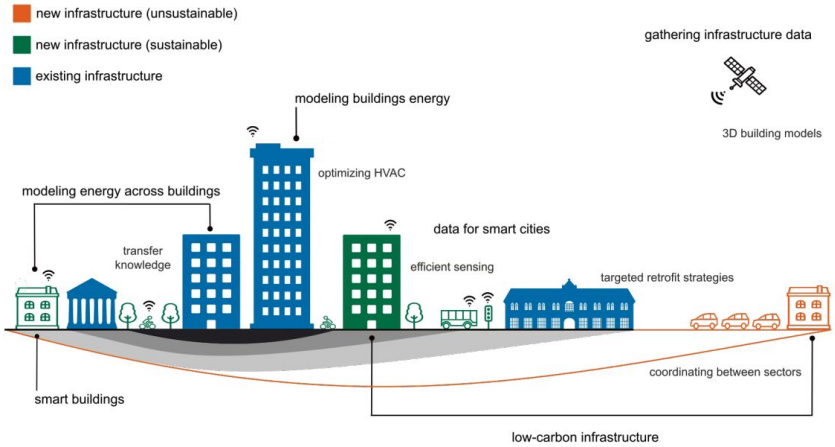


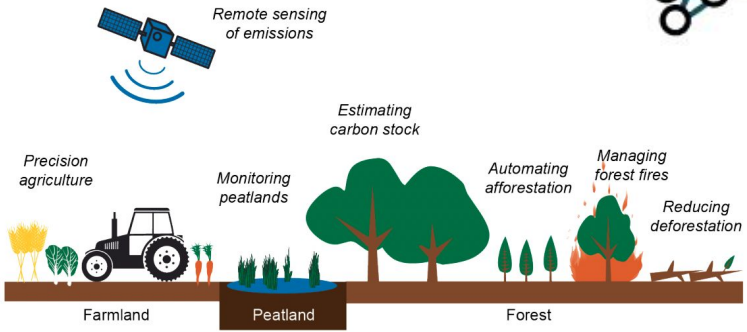
Kiyasseh et al. (2022)

De-biasing surgical AI models with AutoML

Tackling Climate Change with **AutoML**



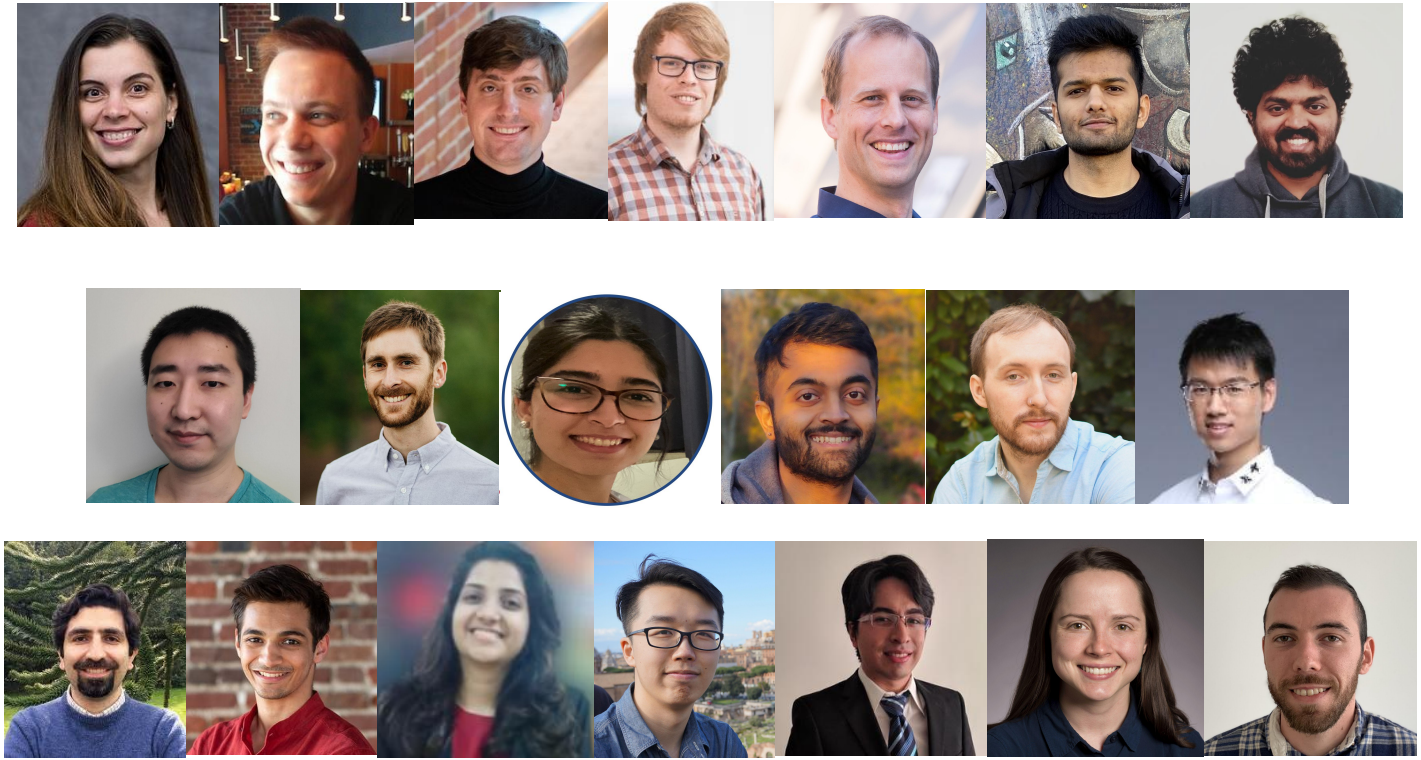




[Rolnick et al. (2018)]

[TRPNJSRTNW (2022)]

Thanks!



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