Does Unsupervised Architecture Representation Learning Help Neural Architecture Search?

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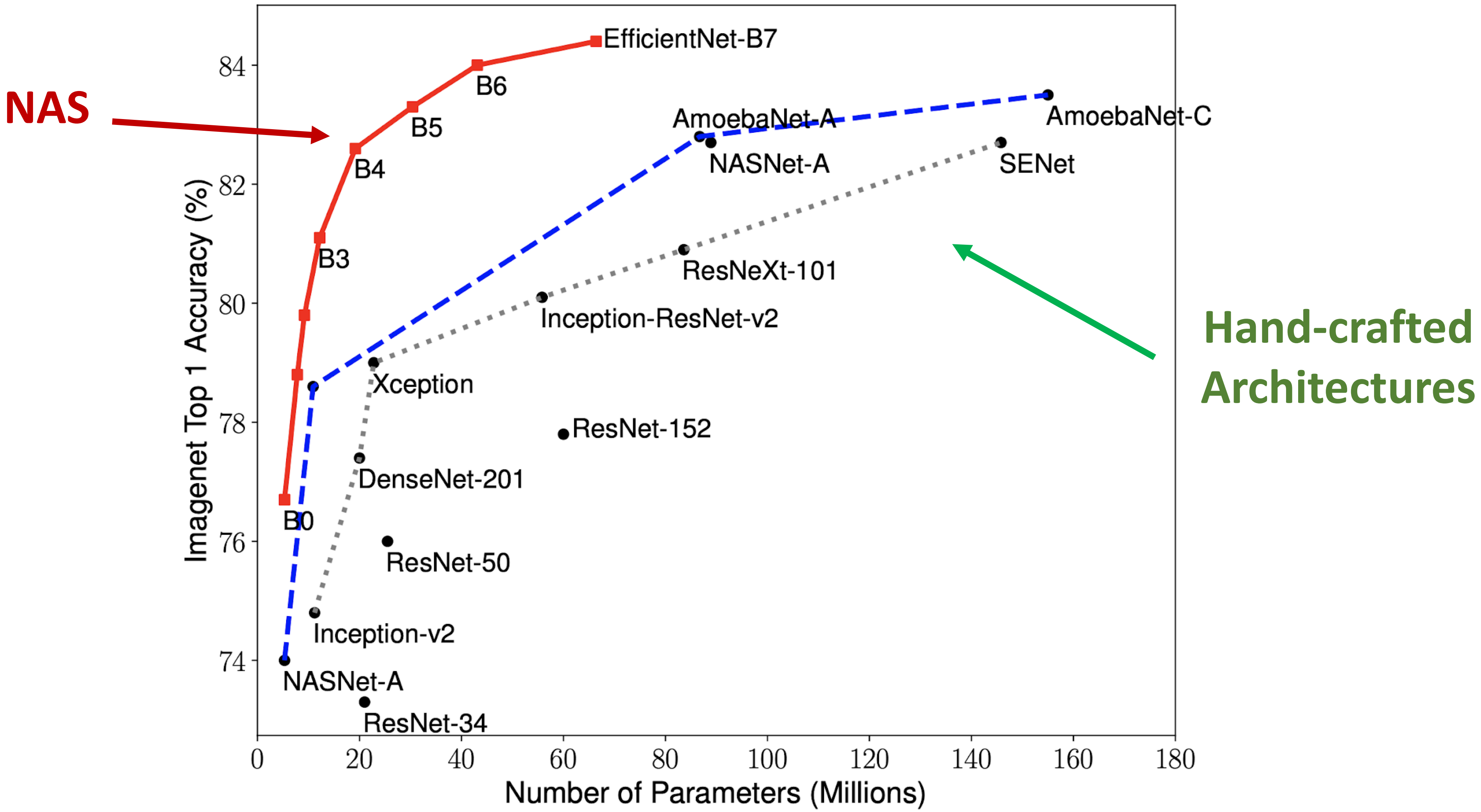
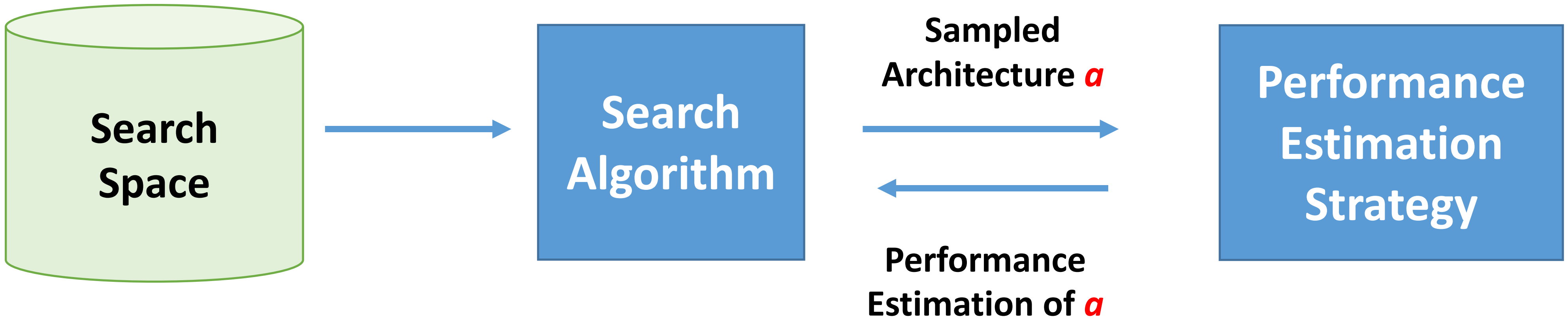
The Rise of Neural Architecture Search (NAS)



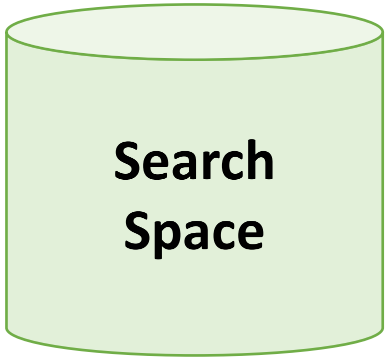
Mingxing Tan, Quoc V. Le, EfficientNet: Rethinking Model Scaling for Convolutional Neural Networks, ICML 2019

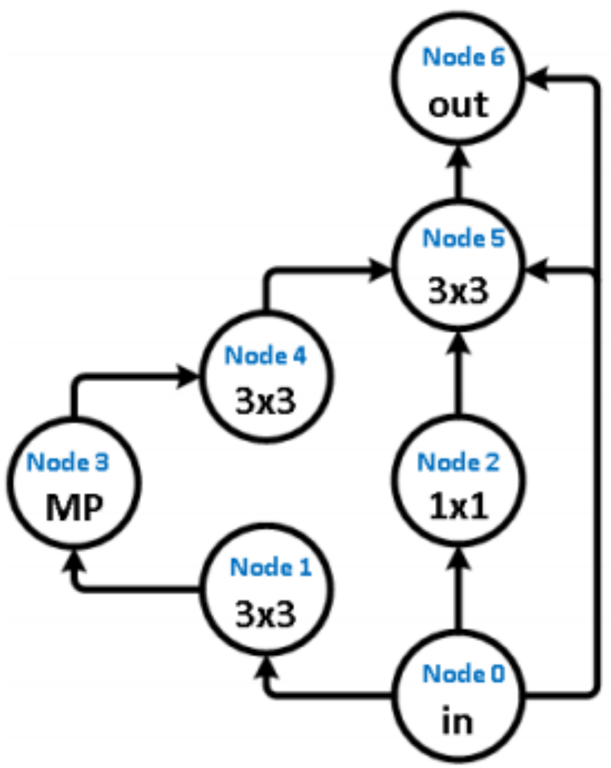
Neural Architecture Search (NAS) Pipeline



Thomas Elsken, Jan Hendrik Metzen, Frank Hutter, Neural Architecture Search: A Survey, JMLR 2019

Search Space



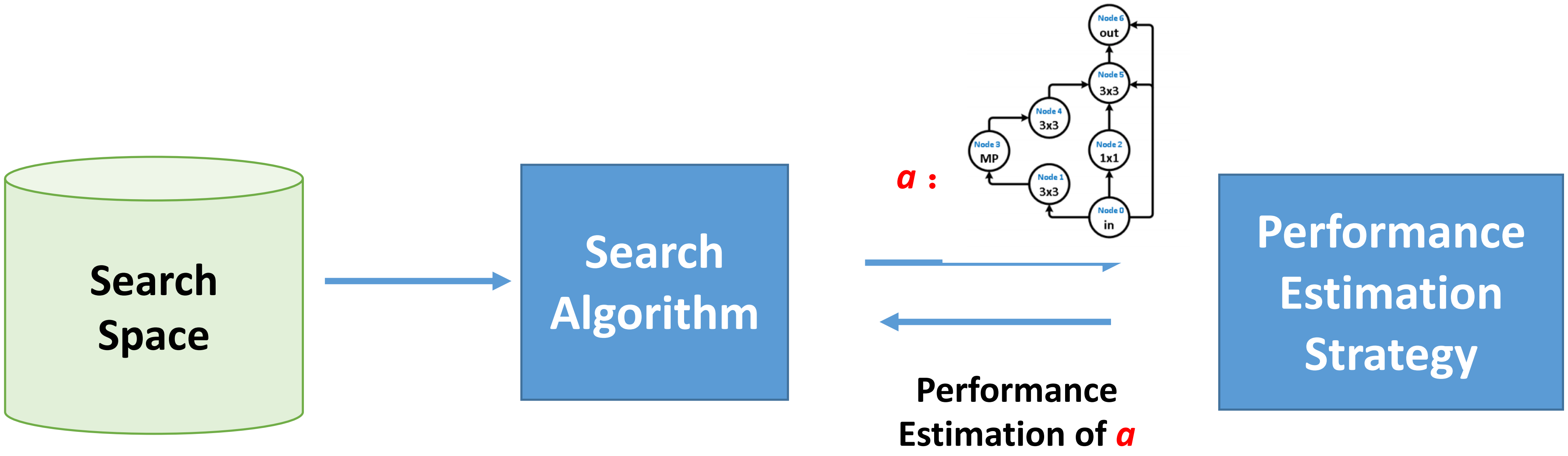


Set of Operations:

- Identity
- avg pooling,
- max pooling,
- standard convolution,
- depthwise-separable convolution.

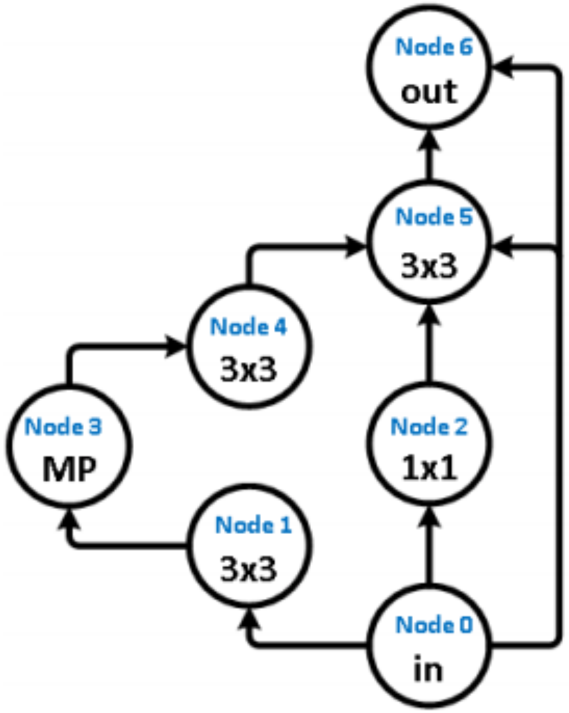
Barret Zoph, Vijay Vasudevan, Jonathon Shlens, Quoc V. Le, Learning Transferable Architectures for Scalable Image Recognition, CVPR 2018

Search Algorithm + Performance Estimation



Evolutionary,
Reinforcement Learning (RL),
Bayesian Optimization (BO)

NAS in Discreate Search Space



Discrete Encoding

Node

$$
\begin{array}{c|c}
 & [0\ \ 1\ \ 2\ \ 3\ \ 4\ \ 5\ \ 6] \\
\text{Node} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix} &
\begin{pmatrix}
0 & 1 & 1 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\end{array}
$$

Adjacency Matrix A

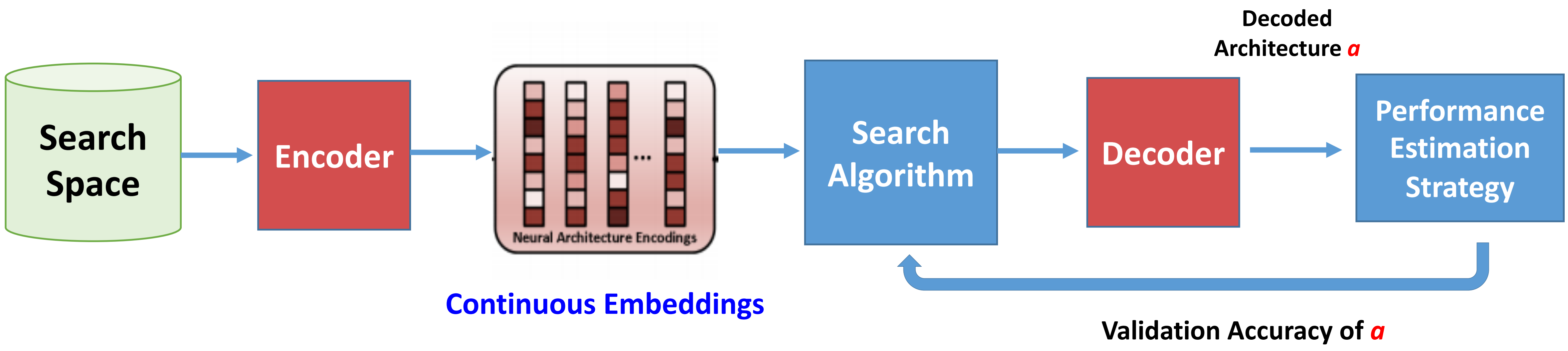
Operation

$$
\begin{array}{c|c}
 & [\text{in}\ \ 1\text{x}1\ \ 3\text{x}3\ \ \text{MP}\ \ \text{out}] \\
\text{Node} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix} &
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}
\end{array}
$$

Operation Matrix X

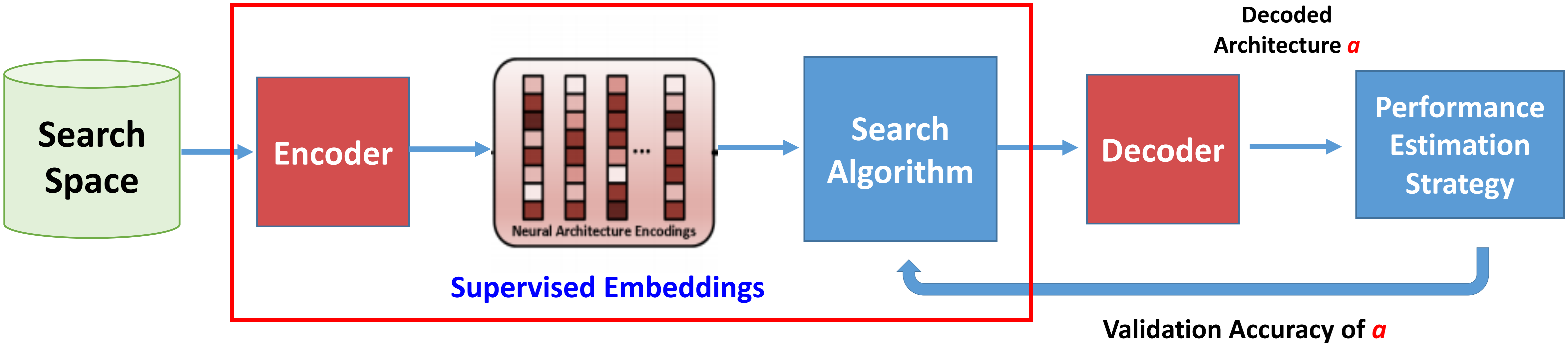
NAS in Continuous Search Space

- Learn continuous embeddings of neural architectures, and perform architecture search in the continuous search space.



NAS in Continuous Search Space

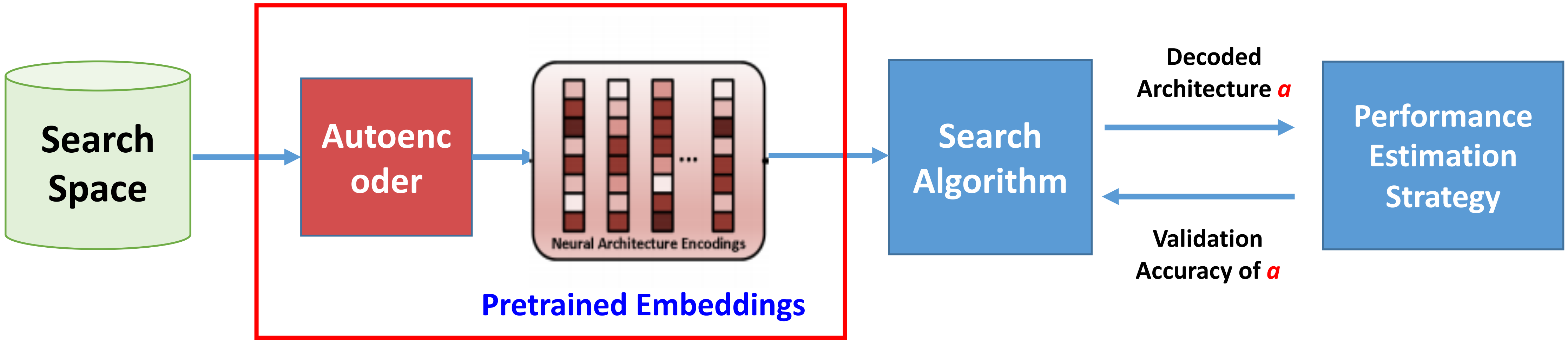
- Architecture embeddings and search strategies are *jointly* optimized in a *supervised* manner, guided by the accuracies of architectures selected by the search strategies.



Architecture embeddings and search strategies are jointly optimized in a supervised manner

Our Contribution

- We propose *arch2vec*, a simple yet effective *unsupervised* architecture representation learning method for neural architecture search.
- *Decouple* architecture embedding learning and architecture search into two *separate* processes.



Pre-training architecture embeddings in an unsupervised manner

Variational Graph Isomorphism Autoencoder

Let **A** denote **Adjacency Matrix**, **X** denote **Operation Matrix**.

Augment **A** as $\tilde{A} = A + A^T$ to transfer original directed graph into undirected one to allow bi-directional information flow.

Encoder

$$q(\mathbf{Z}|\mathbf{X}, \tilde{\mathbf{A}}) = \prod_{i=1}^{N} q(\mathbf{z}_i|\mathbf{X}, \tilde{\mathbf{A}}), \text{with } q(\mathbf{z}_i|\mathbf{X}, \tilde{\mathbf{A}}) = \mathcal{N}(\mathbf{z}_i|\boldsymbol{\mu}_i, diag(\boldsymbol{\sigma}_i^2)),$$

$$\mathbf{H}^{(k)} = \mathrm{MLP}^{(k)}\left(\left(1 + \epsilon^{(k)}\right) \cdot \mathbf{H}^{(k-1)} + \tilde{\mathbf{A}}\mathbf{H}^{(k-1)}\right), k = 1, 2, \ldots, L$$

L-layer Graph Isomorphism Network (GIN)

Decoder

$$p(\hat{\mathbf{A}}|\mathbf{Z}) = \prod_{i=1}^{N}\prod_{j=1}^{N} P(\hat{A}_{ij}|\mathbf{z}_i, \mathbf{z}_j), \text{with } p(\hat{A}_{ij} = 1|\mathbf{z}_i, \mathbf{z}_j) = \sigma(\mathbf{z}_i^T\mathbf{z}_j)$$

Reconstructed Adjacency Matrix

$$p(\hat{\mathbf{X}} = [k_1, \ldots, k_N]^T|\mathbf{Z}) = \prod_{i=1}^{N} P(\hat{\mathbf{X}}_i = k_i|\mathbf{z}_i) = \prod_{i=1}^{N} \mathrm{softmax}(\mathbf{W}_o\mathbf{Z} + \mathbf{b}_o)_{i,k_i}$$

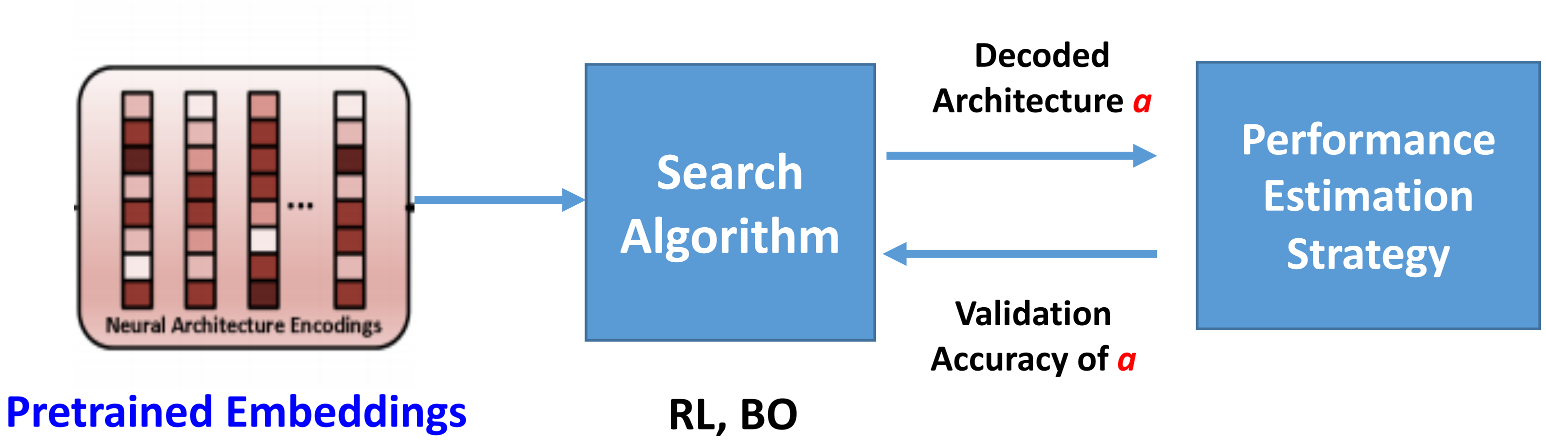
Reconstructed Operation Matrix

Training objective

$$\mathcal{L} = \mathbb{E}_{q(\mathbf{Z}|\mathbf{X},\tilde{\mathbf{A}})}[\log p(\hat{\mathbf{X}}, \hat{\mathbf{A}}|\mathbf{Z})] - \mathcal{D}_{KL}(q(\mathbf{Z}|\mathbf{X}, \tilde{\mathbf{A}})||p(\mathbf{Z}))$$

Pretrained Embeddings for Architecture Search

We use reinforcement learning (RL) and Bayesian optimization (BO) as two representative search algorithms.



Pre-training Performance

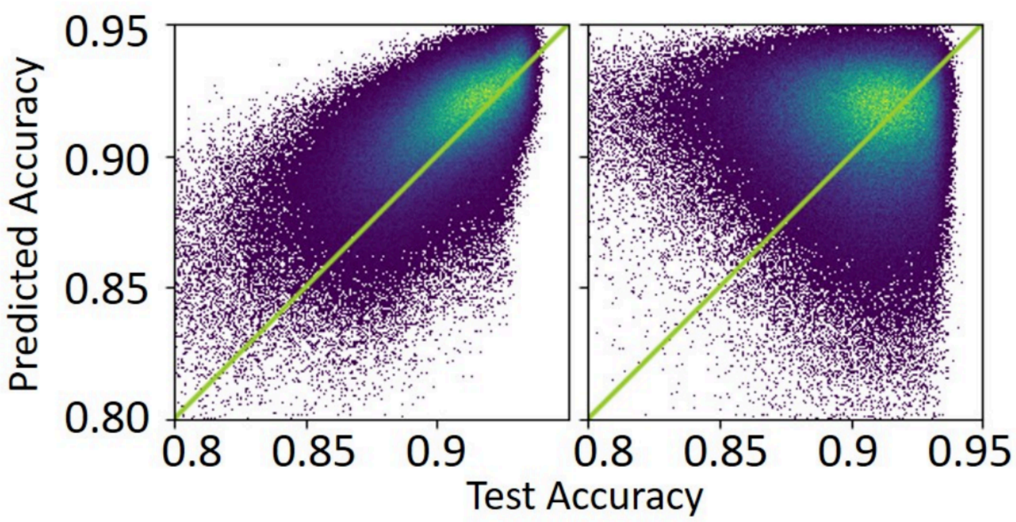
- Three commonly used NAS search spaces: **NAS-Bench-101**, **NAS-Bench-201**, and the **DARTS** search space.
- We compare *arch2vec* with two baselines: Graph Autoencoders (GAE) and Variational Graph Autoencoders (VGAE) under three metrics:
    - **Reconstruction Accuracy**: how accurate the reconstructed network architectures are.
    - **Validity**: how often the generated architectures are valid.
    - **Uniqueness**: how many generated valid architectures are unique.

Method	NAS-Bench-101			NAS-Bench-201			DARTS		
	Accuracy	Validity	Uniqueness	Accuracy	Validity	Uniqueness	Accuracy	Validity	Uniqueness
GAE [27]	98.75	29.88	99.25	99.52	79.28	78.42	97.80	15.25	99.65
VGAE [27]	97.45	41.18	99.34	98.32	79.30	88.42	96.80	25.25	99.27
arch2vec	**100**	**51.33**	**99.36**	**100**	**79.41**	**98.72**	**99.79**	**33.36**	**100**

Understanding the Superiority of Pretrained Embeddings (1)

- We compare the predictive performance of the pretrained embeddings and supervised embeddings. This metric measures how well the embeddings can predict the performance of the corresponding architectures.

- We train a Gaussian Process model with 250 sampled data to predict all data and report the results across 10 different seeds. We use RMSE and the Pearson correlation coefficient to evaluate points with test accuracy larger than 0.8.



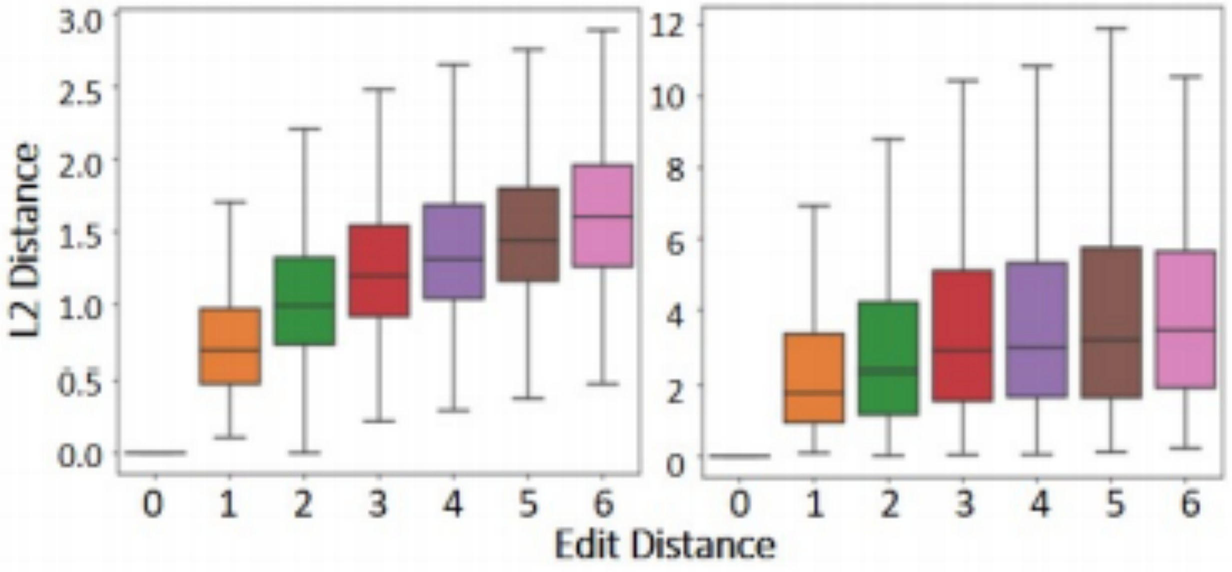
Pretrained Embeddings (i.e., our approach)

Supervised Embeddings

The RMSE and Pearson's r are: 0.038±0.025 / 0.53±0.09 for supervised embeddings, and 0.018±0.001 / 0.67±0.02 for *arch2vec*.

Understanding the Superiority of Pretrained Embeddings (2)

- We compare the distribution of L2 distance between architecture pairs by edit distance, measured by 1,000 architectures sampled in a long random walk with 1 edit distance apart from consecutive samples.
- The L2 distance of pretrained embeddings grows monotonically with increasing edit distance.
- This observation indicates that the pretrained embeddings are able to better capture the structural information of neural networks, and thus make similar architectures clustered better.

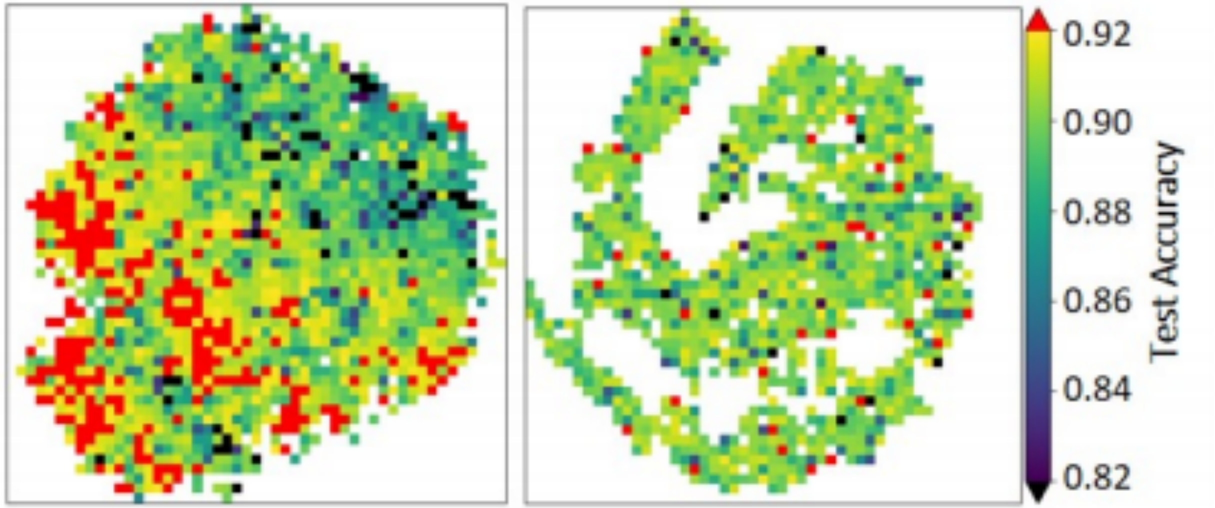


Pretrained Embeddings (i.e., our approach)

Supervised Embeddings

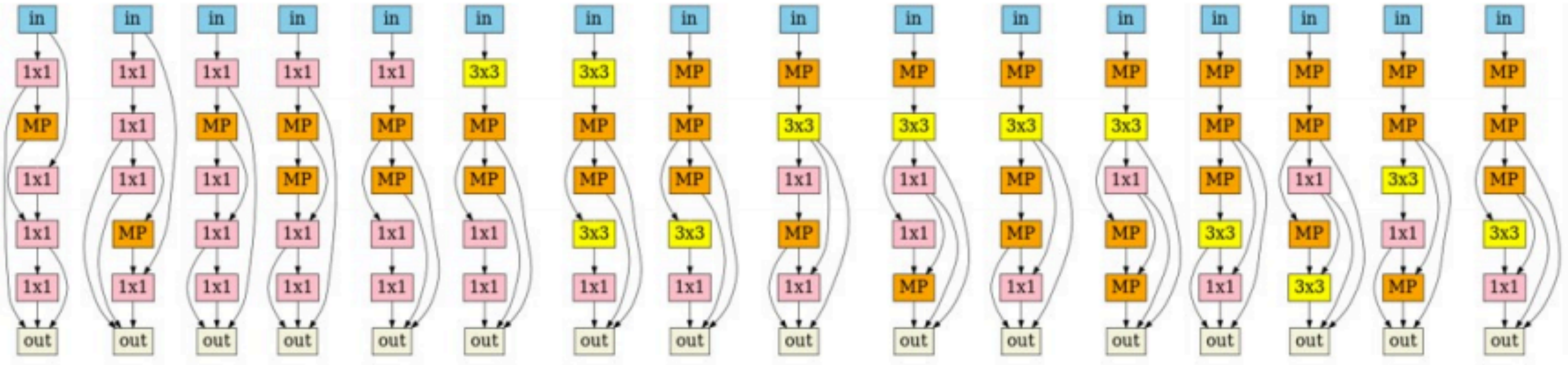
Understanding the Superiority of Pretrained Embeddings (3)

- We visualize the latent spaces learned by *arch2vec* and its supervised learning counterpart in 2-dimensional space.
- Compared to supervised embeddings, pretrained embeddings span the whole latent space, and architectures with similar accuracies are clustered and distributed more smoothly in the latent space.
- Conducting architecture search on such smooth performance surface is much easier and is hence more efficient.

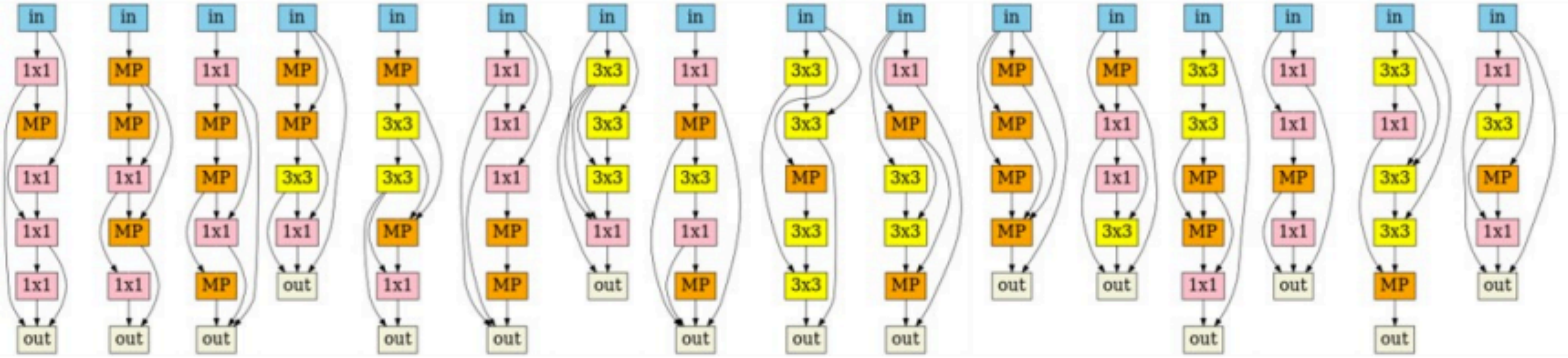


Latent space 2D visualization comparison between arch2vec (left) and supervised architecture representation learning (right). Color encodes test accuracy.

Understanding the Superiority of Pretrained Embeddings (4)



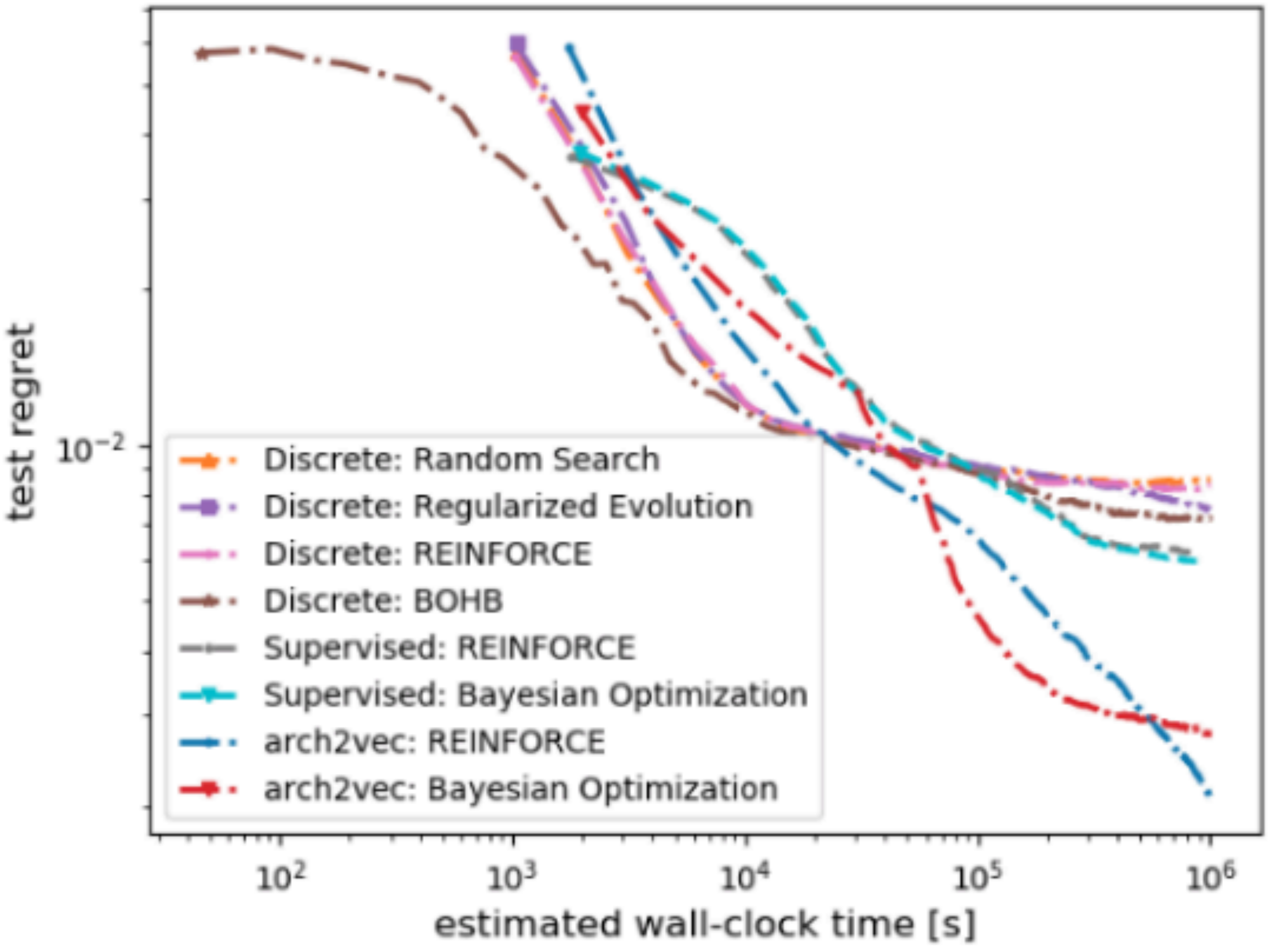
Pretrained Embeddings (edit distances between adjacent architectures are 4, 6, 1, 5, 1, 1, 1, 5, 2, 3, 2, 4, 2, 5, 2;)



Supervised Embeddings (edit distances between adjacent architectures are 8, 6, 7, 7, 9, 8, 11, 11, 6, 10, 10, 11, 10, 11, 9)

Architecture Search Performance on NAS-Bench-101

- BOHB and RE are two best-performing search methods using discrete encoding.
- However, they perform slightly worse than supervised architecture representation learning.
- *arch2vec* considerably outperforms its supervised counterpart and the discrete encoding after 5 × 10^4 wall clock seconds.



Architecture Search Performance on NAS-Bench-201

- Searching with *arch2vec* consistently outperforms other approaches on all the three datasets in NAS-Bench-201, leading to better validation and test accuracy as well as reduced variability.

NAS Methods	**CIFAR-10**		**CIFAR-100**		**ImageNet-16-120**	
	validation	test	validation	test	validation	test
RE [41]	91.08±0.43	93.84±0.43	73.02±0.46	72.86±0.55	45.78±0.56	45.63±0.64
RS [59]	90.94±0.38	93.75±0.37	72.17±0.64	72.05±0.77	45.47±0.65	45.33±0.79
REINFORCE [10]	91.03±0.33	93.82±0.31	72.35±0.63	72.13±0.79	45.58±0.62	45.30±0.86
BOHB [12]	90.82±0.53	93.61±0.52	72.59±0.82	72.37±0.90	45.44±0.70	45.26±0.83
arch2vec-RL	91.32±0.42	94.12±0.42	73.13±0.72	73.15±0.78	46.22±0.30	46.16±0.38
arch2vec-BO	**91.41±0.22**	**94.18±0.24**	**73.35±0.32**	**73.37±0.30**	**46.34±0.18**	**46.27±0.37**

Architecture Search Performance on DARTS search space

- *arch2vec* leads to competitive search performance among different cell-based NAS methods with comparable model parameters.

	Test Error		Params (M)	Search Cost				
NAS Methods	Avg	Best		Stage 1	Stage 2	Total	**Encoding**	**Search Method**
Random Search [15]	3.29±0.15	-	3.2	-	-	4	-	Random
ENAS [61]	-	2.89	4.6	0.5	-	-	Supervised	REINFORCE
ASHA [62]	3.03±0.13	2.85	2.2	-	-	9	-	Random
RS WS [62]	2.85±0.08	2.71	4.3	2.7	6	8.7	-	Random
SNAS [16]	2.85±0.02	-	2.8	1.5	-	-	Supervised	GD
DARTS [15]	2.76±0.09	-	3.3	4	1	5	Supervised	GD
BANANAS [43]	2.64	2.57	3.6	100 (queries)	-	11.8	Supervised	BO
Random Search (ours)	3.1±0.18	2.71	3.2	-	-	4	-	Random
DARTS (ours)	2.71±0.08	2.63	3.3	4	1.2	5.2	Supervised	GD
BANANAS (ours)	2.67±0.07	2.61	3.6	100 (queries)	1.3	11.5	Supervised	BO
arch2vec-RL	2.65±0.05	2.60	3.3	100 (queries)	1.2	9.5	Unsupervised	REINFORCE
arch2vec-BO	**2.56±0.05**	**2.48**	3.6	100 (queries)	1.3	10.5	Unsupervised	BO

For more detailed information and other results, please refer to our paper:
https://arxiv.org/abs/2006.06936

Thank You