Neural Architecture Search (part 1)

Motivation

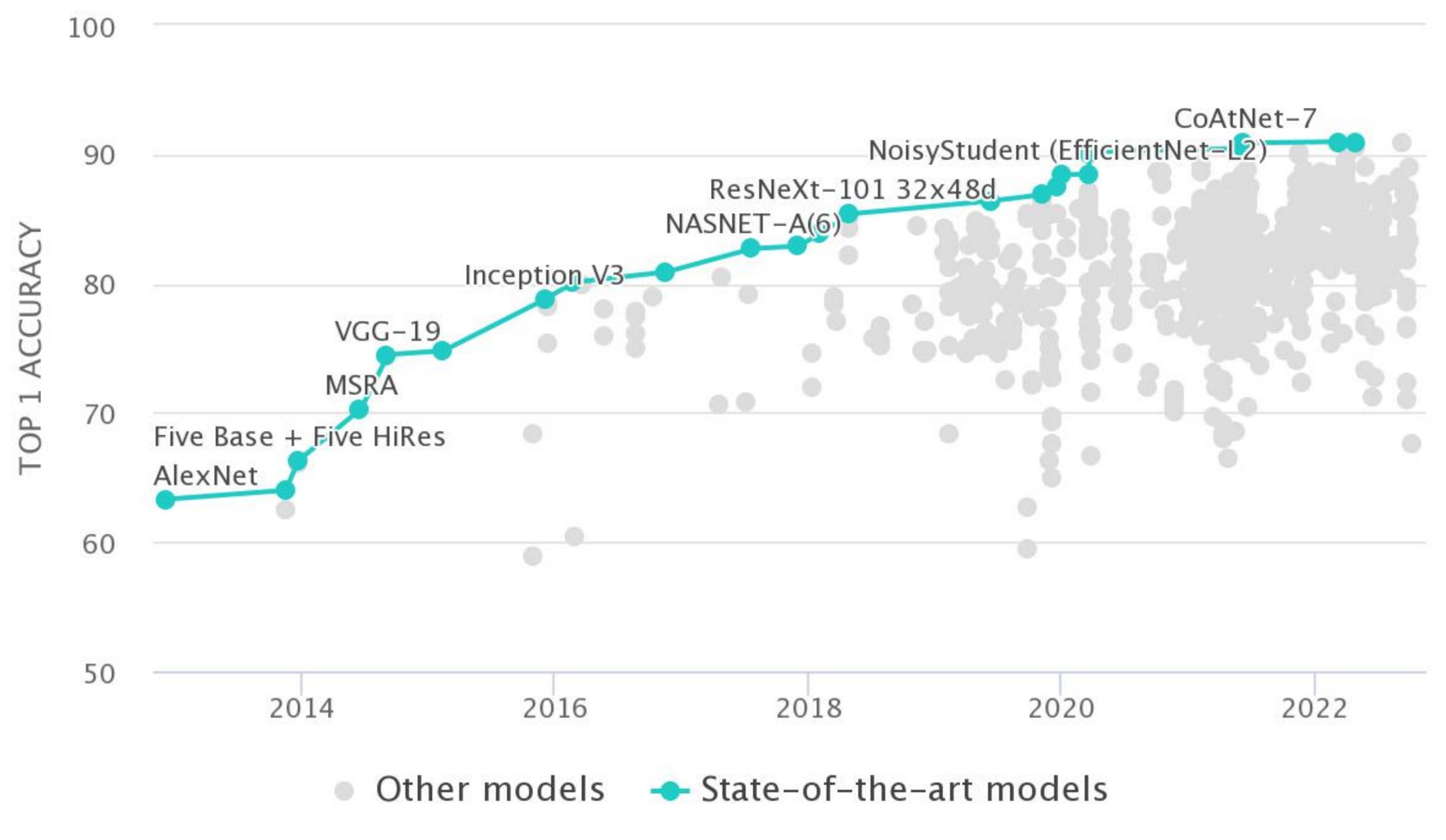
	1 _	1 -	I	l	l	
Input	Operator	exp size	$\mid \#out \mid$	SE	NL	s
$224^2 \times 3$	conv2d	_	16	_	HS	2
$112^2 \times 16$	bneck, 3x3	16	16	_	RE	1
$112^{2} \times 16$	bneck, 3x3	64	24	_	RE	2
$56^2 \times 24$	bneck, 3x3	72	24	_	RE	1
$56^2 \times 24$	bneck, 5x5	72	40	✓	RE	2
$28^2 \times 40$	bneck, 5x5	120	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
$7^2 imes 960$	pool, 7x7	_	_	_	_	1
$1^{2} \times 960$	conv2d 1x1, NBN	_	1280	_	HS	1
$1^2 \times 1280$	conv2d 1x1, NBN	-	k	-	-	1

Table 1. Specification for MobileNetV3-Large. SE denotes whether there is a Squeeze-And-Excite in that block. NL denotes the type of nonlinearity used. Here, HS denotes h-swish and RE denotes ReLU. NBN denotes no batch normalization. s denotes stride.

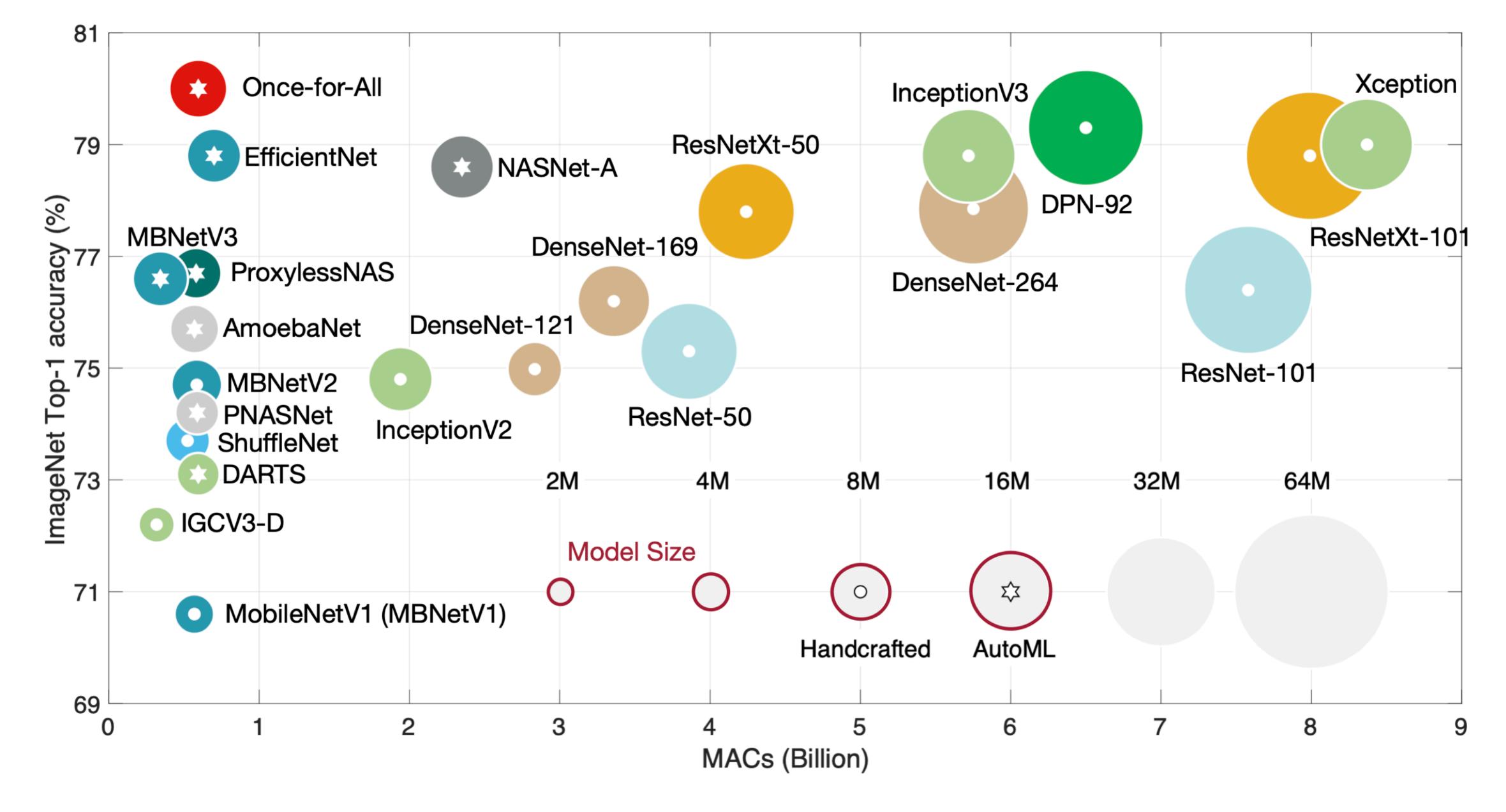
Today's NN architectures are very carefully designed! There are so many things that we can tune:

 Number of Layers 	#
 #channels in each layer 	# [
 Activation function for each layer 	# Swish? ReLU? GeLU?
 Type of the operator 	# bottleneck? conv2d? else?
 Kernel size 	# 3x3? 5x5? 7x7?
 Where to downsample? 	#
 How to downsample? 	# Stride? Pool?
 Overall topology 	# Recurrent? Skip-connect?

Large Search Space? Let Machine do it!



2017. Machine-tuned networks already took over in terms of test accuracy



2020. Machine-tuned networks are dominant in terms of compute-efficiency.

Neural Architecture Search

You search over the space of possible NN architectures, and try to look for the best one.

Dumb Strategy. Here is a dumb way to do it (brute-force search).

- List up all design hyperparameters and determine their range
- Make a lot of NN by combining all possible choices of hyperparameters
 # Exponential growth

No restriction

• Fully train each network until convergence, and select the best-performing one. # Much compute

Question. What is a better strategy?

Revisit the dumb strategy...

List up all design hyperparameters and determine their range

- 1. Well-designed Search Space
- Make a lot of NN by combining all possible choices of hyperparameters

- 2. Smarter Exploration
- Fully train each network until convergence, and select the best-performing one. 3. Cheaper evaluation

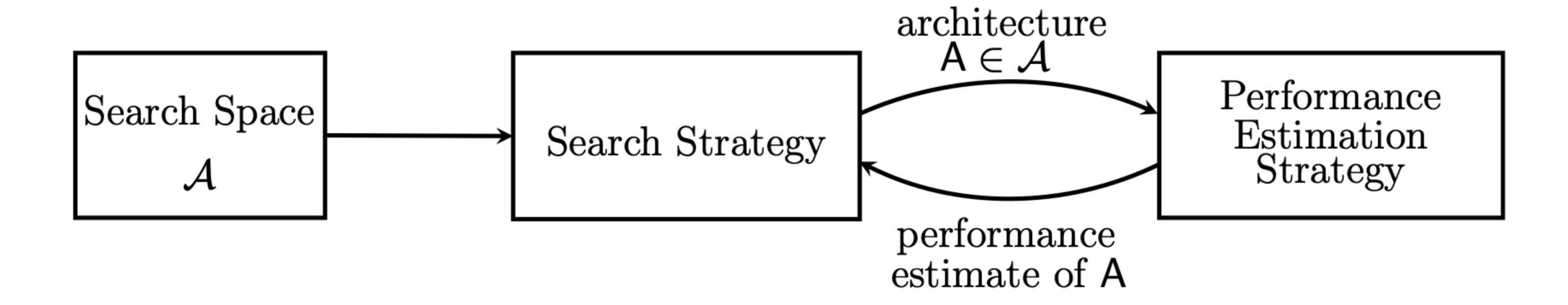
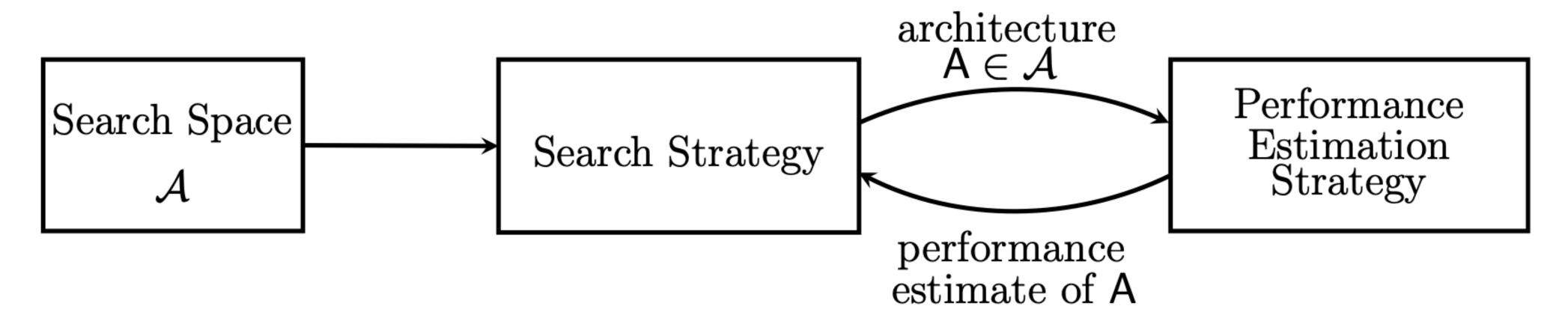
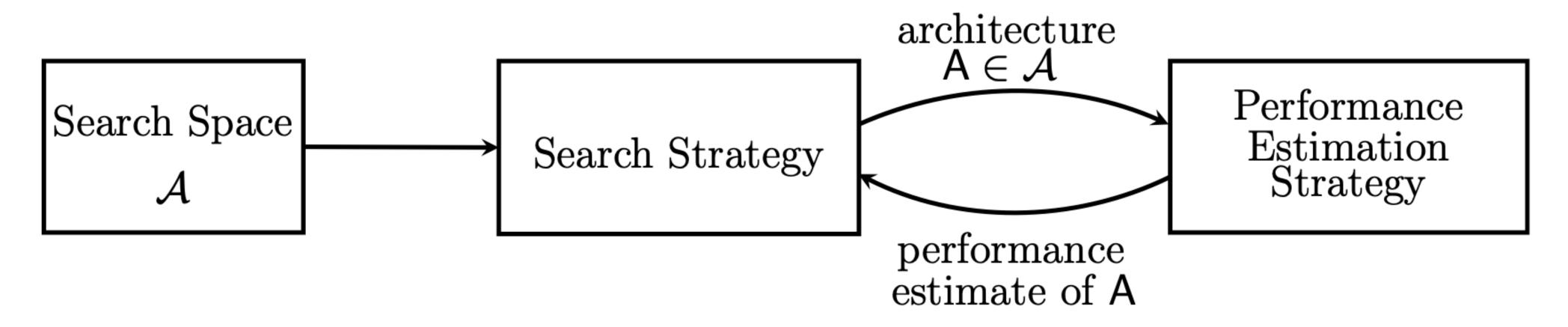


Figure 1: Abstract illustration of Neural Architecture Search methods. A search strategy selects an architecture A from a predefined search space \mathcal{A} . The architecture is passed to a performance estimation strategy, which returns the estimated performance of A to the search strategy.



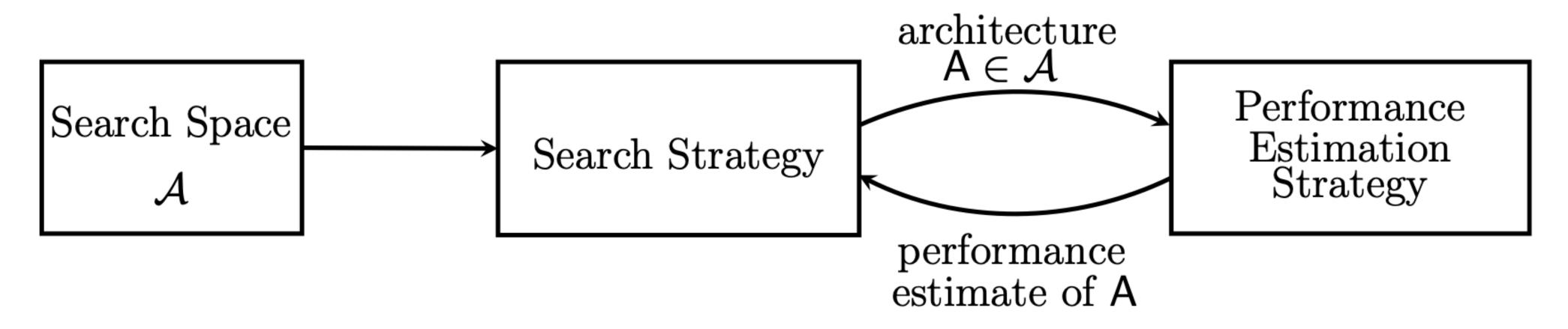
Search Space.

- Defines which architectures can be represented in principle.
- Can be reduced in size, by incorporating prior knowledge about typical properties of architectures well-suited for a task (e.g., convolution for vision)
 - But this introduce human bias; better to avoid if we have enough compute.



Search Strategy.

- Details how to explore the search space.
 (Can be exponentially large or unbounded)
- Encompasses the classical exploration-exploitation trade-off
 - Desirable to find well-performing architecture quickly
 - Premature convergence to a region of suboptimal architecture should be avoided



Performance Estimation Strategy.

- Estimate the predictive performance of a model.
- Simplest: to perform a standard training and measure validation performance
 - Too expensive
- Much efforts made in reducing the cost.

An Elementary Form

To give you an idea, here is an elementary version of neural architecture search:

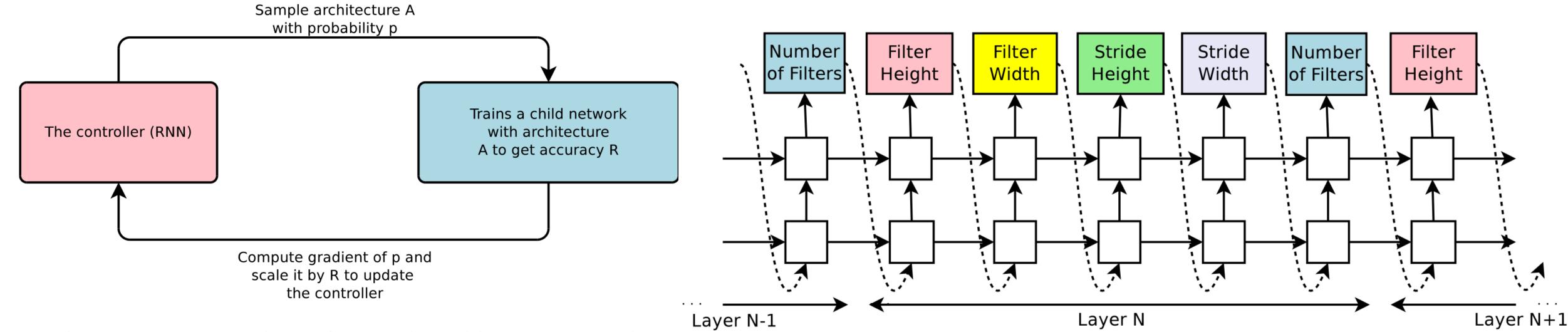


Figure 1: An overview of Neural Architecture Search.

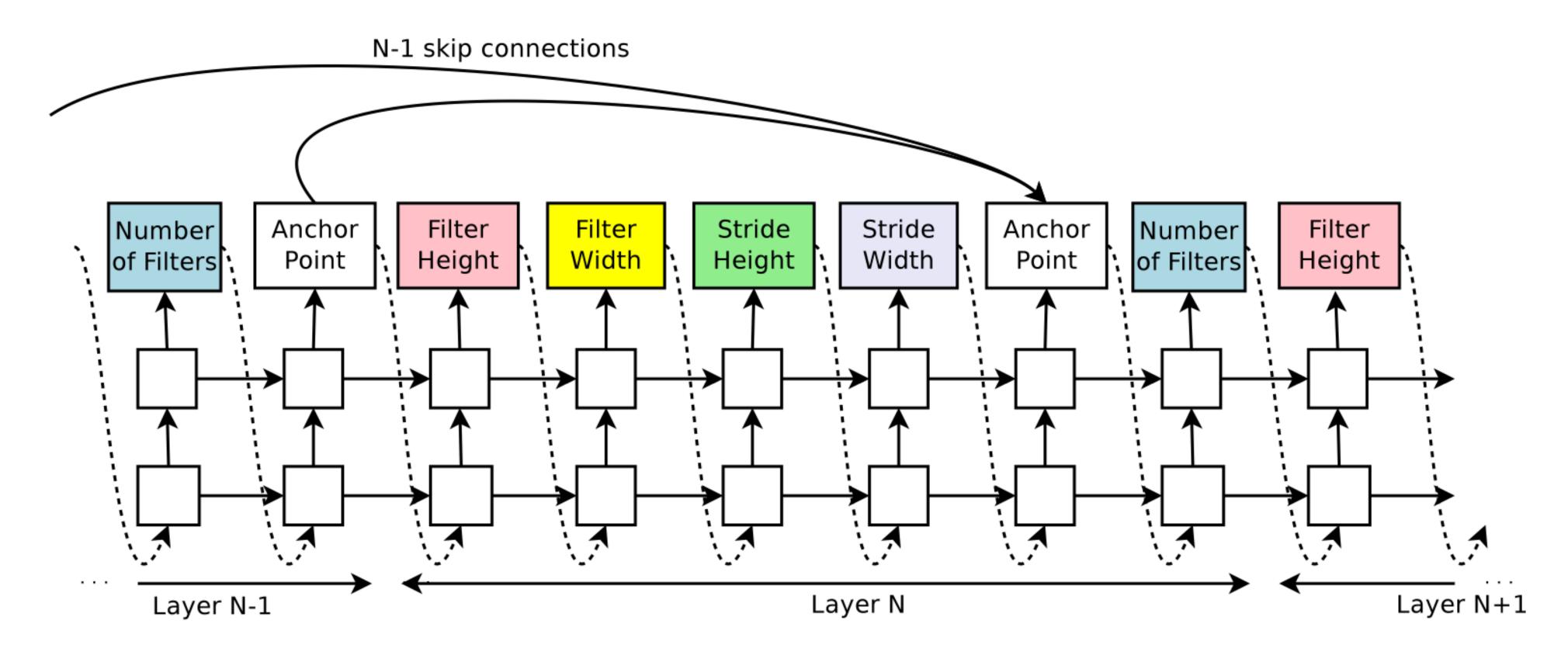
- Search Space: Convolutional neural network with L layers.
- Search Strategy: Reinforcement Learning with RNN controller (policy); reward given by the performance
- **Performance Estimation:** Train for *t* steps

Let's tackle each of these separately...

Search Space

A simplest method construct the search space is to view NN as a sequence of layers (forget about topologies), and predict the HP for each layer separately — first predict type, and predict relevant parameters.

Example. Zoph and Le (2017) constrains the search space to a fully convolutional network, and aim to predict #filters / kernel size / strides / residuals (and do additional tricks, too)



Predicting all parameters separately is a tedious thing to do—Zoph and Le (2017) uses 800 GPUs for 28 days!

Cell-based representation. Same cell (also called *motifs*) may be used repeatedly as a block.

(This is quite common in successful in handcrafted nets, so why not?)

- Reduces the search space—less effort for search
- Known to have better transferrability across tasks

NASNet (Zoph et al., 2018) organizes the layers into multiple groups of normal / reduction cells, and try to learn how each normal / reduction cell should look like.

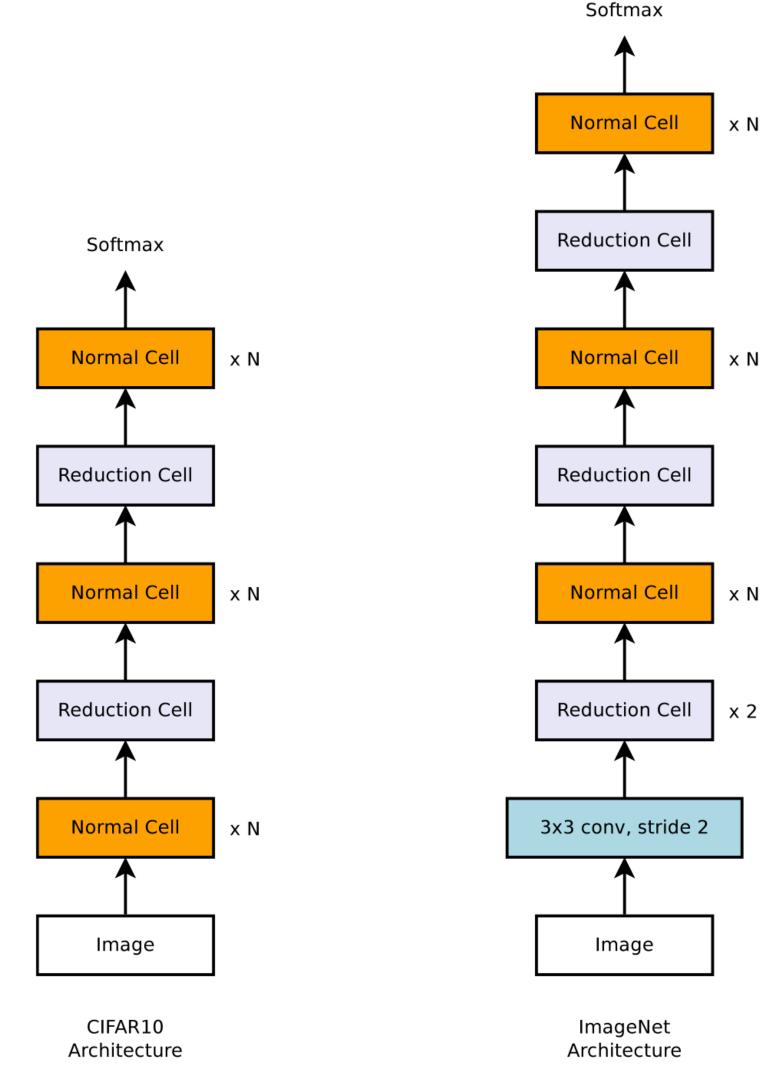
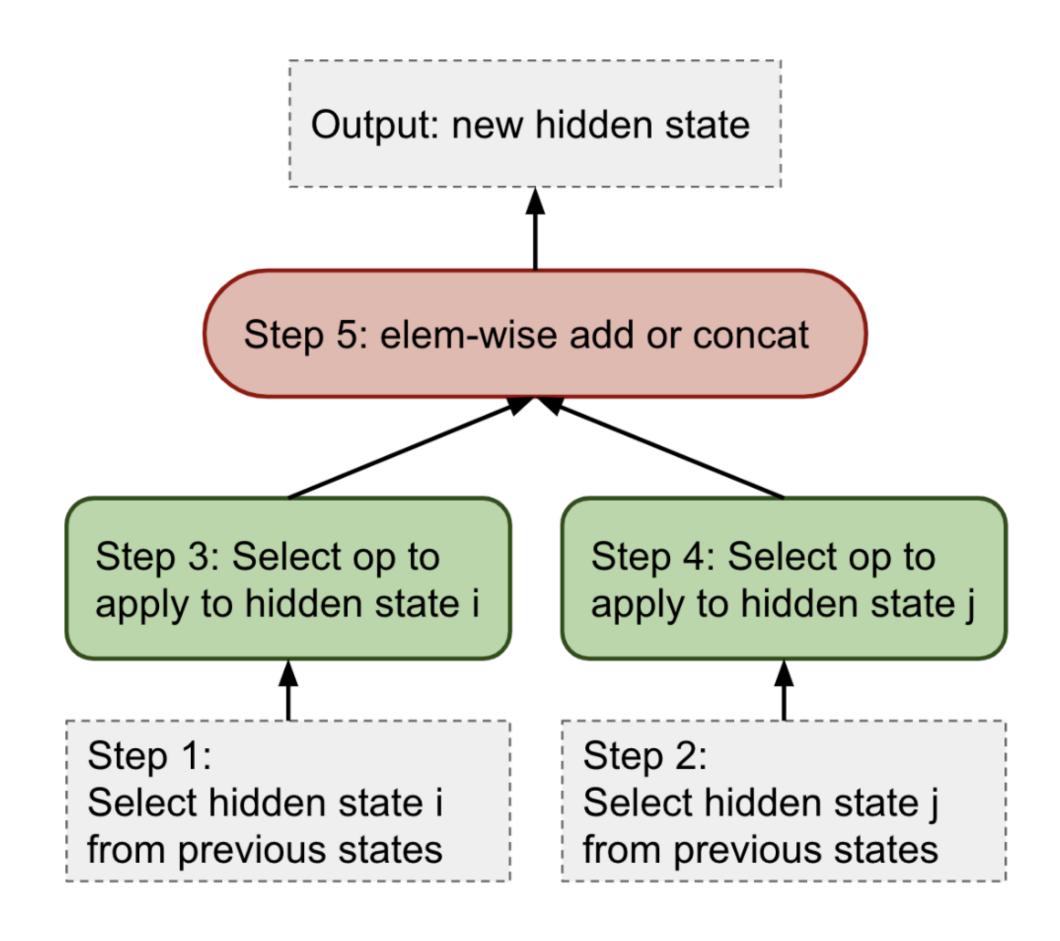


Figure 2. Scalable architectures for image classification consist of two repeated motifs termed $Normal\ Cell$ and $Reduction\ Cell$. This diagram highlights the model architecture for CIFAR-10 and ImageNet. The choice for the number of times the Normal Cells that gets stacked between reduction cells, N, can vary in our experiments.

Each cell consists of B=5 blocks.

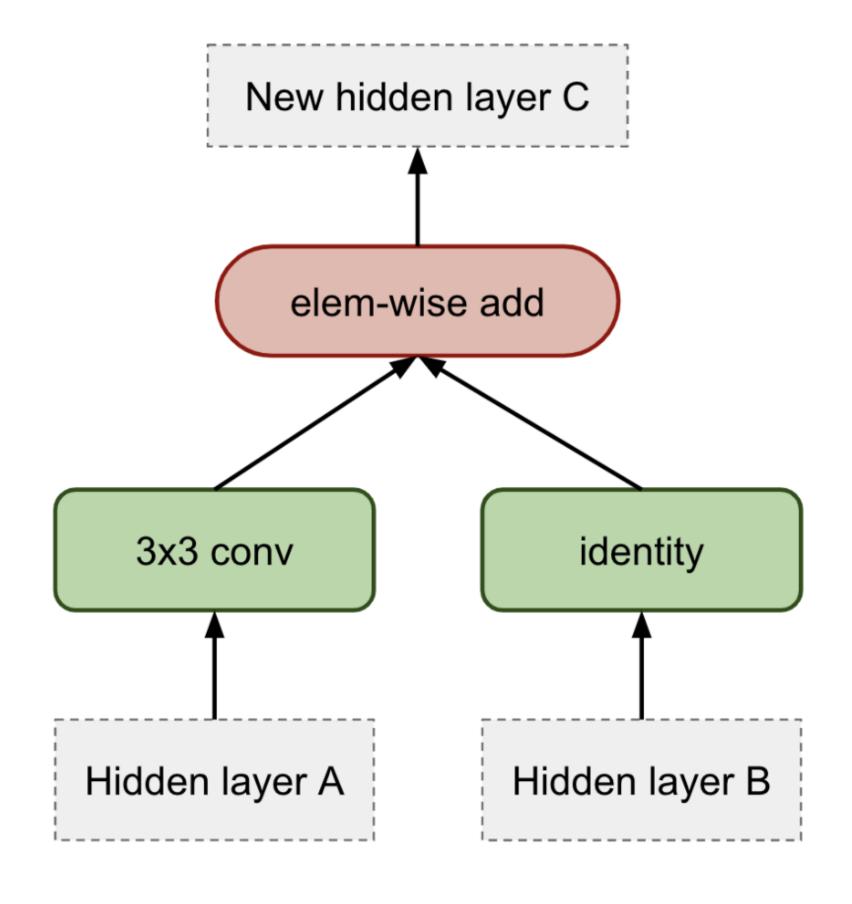
Adding each block requires a five-step decision. (We use RNN to make five decisions sequentially)



(a) 5 discrete choices in each block

- identity
- 1x7 then 7x1 convolution
- 3x3 average pooling
- 5x5 max pooling
- 1x1 convolution
- 3x3 depthwise-separable conv
- 7x7 depthwise-separable conv

- 1x3 then 3x1 convolution
- 3x3 dilated convolution
- 3x3 max pooling
- 7x7 max pooling
- 3x3 convolution
- 5x5 depthwise-seperable conv



(b) A concrete example

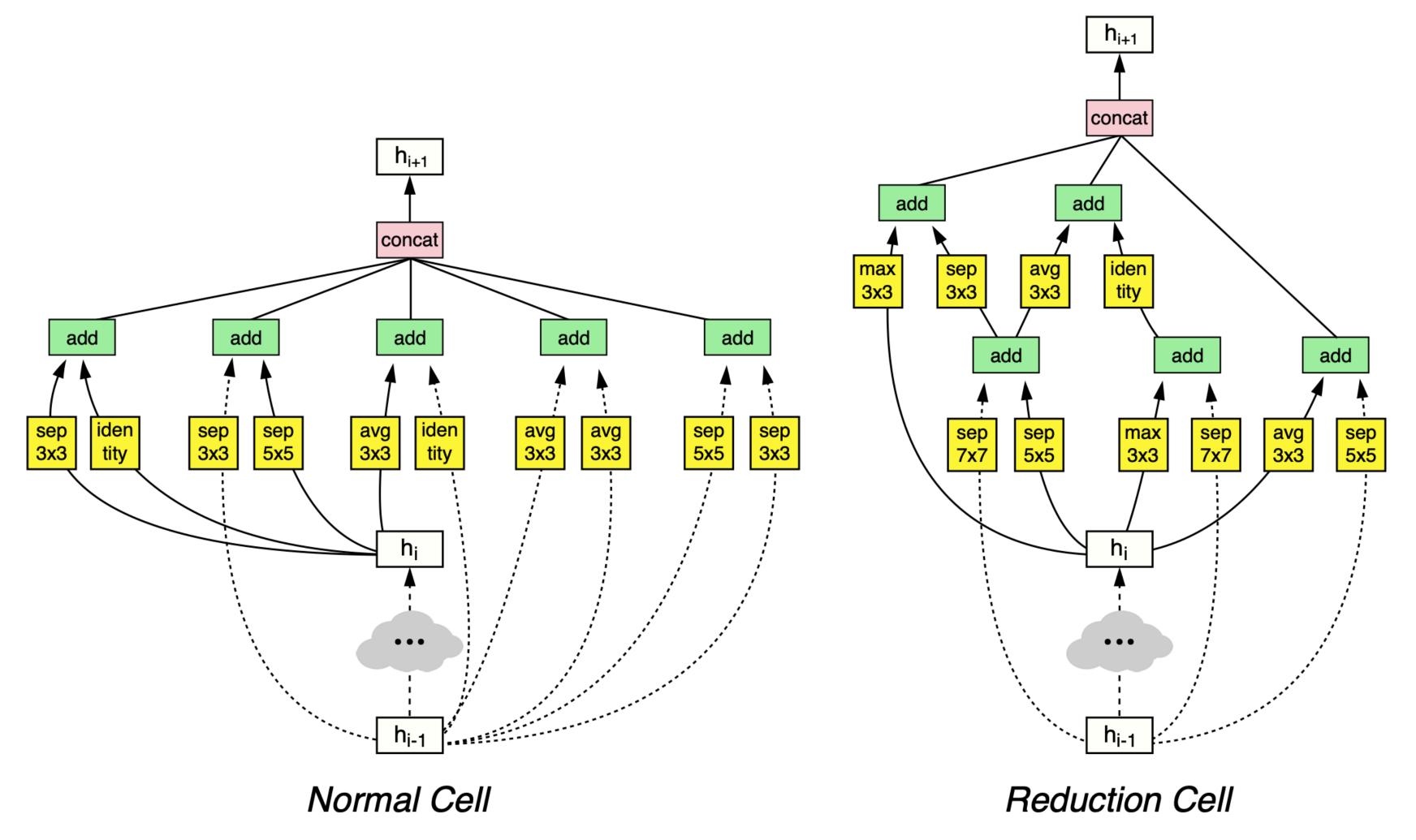
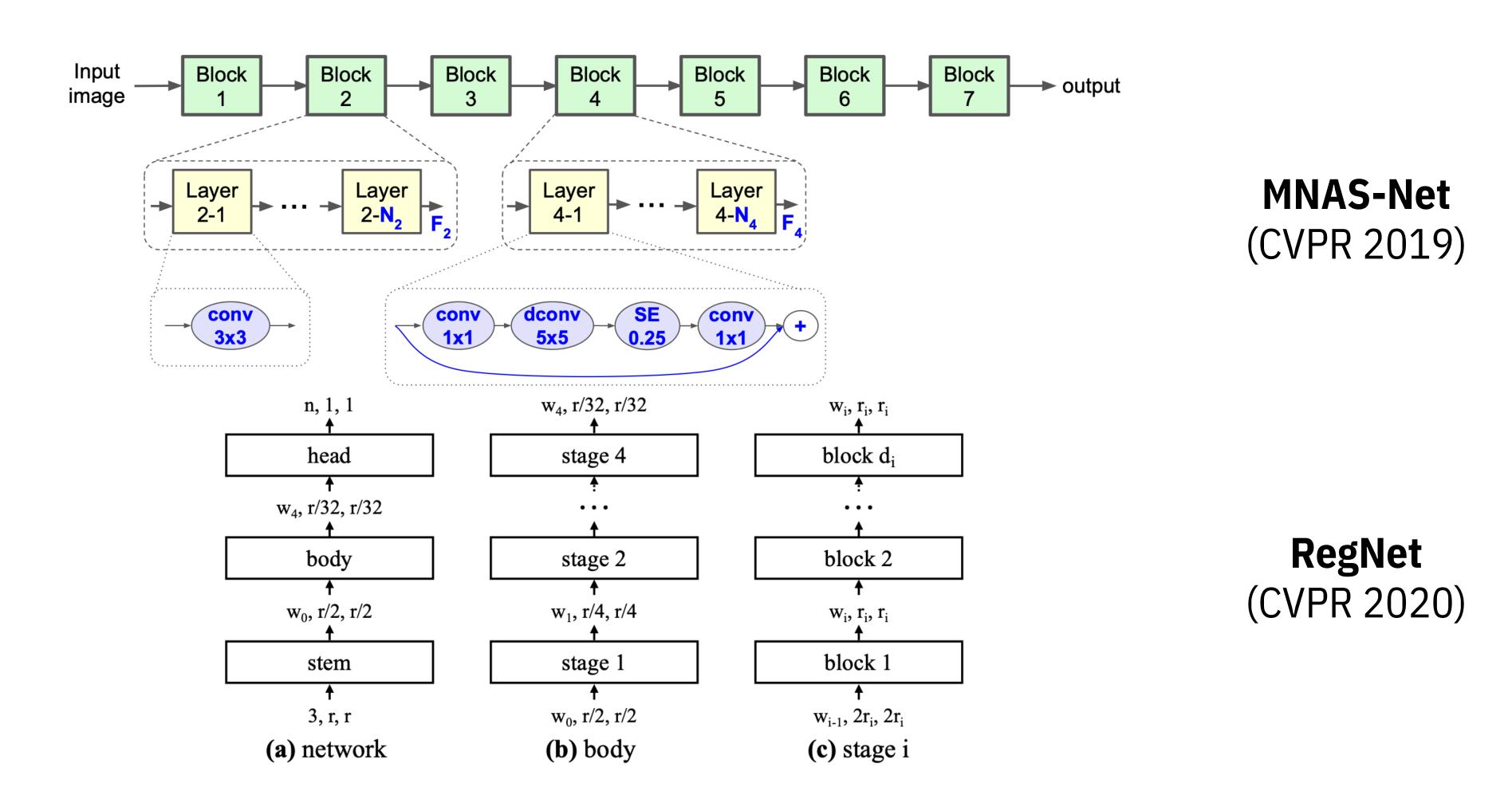


Figure 4. Architecture of the best convolutional cells (NASNet-A) with B=5 blocks identified with CIFAR-10. The input (white) is the hidden state from previous activations (or input image). The output (pink) is the result of a concatenation operation across all resulting branches. Each convolutional cell is the result of B blocks. A single block is corresponds to two primitive operations (yellow) and a combination operation (green). Note that colors correspond to operations in Figure 3.

Search Space, with topologies

In previous examples, we can only change a very limited number of things at a network-level (⇔ cell-level)

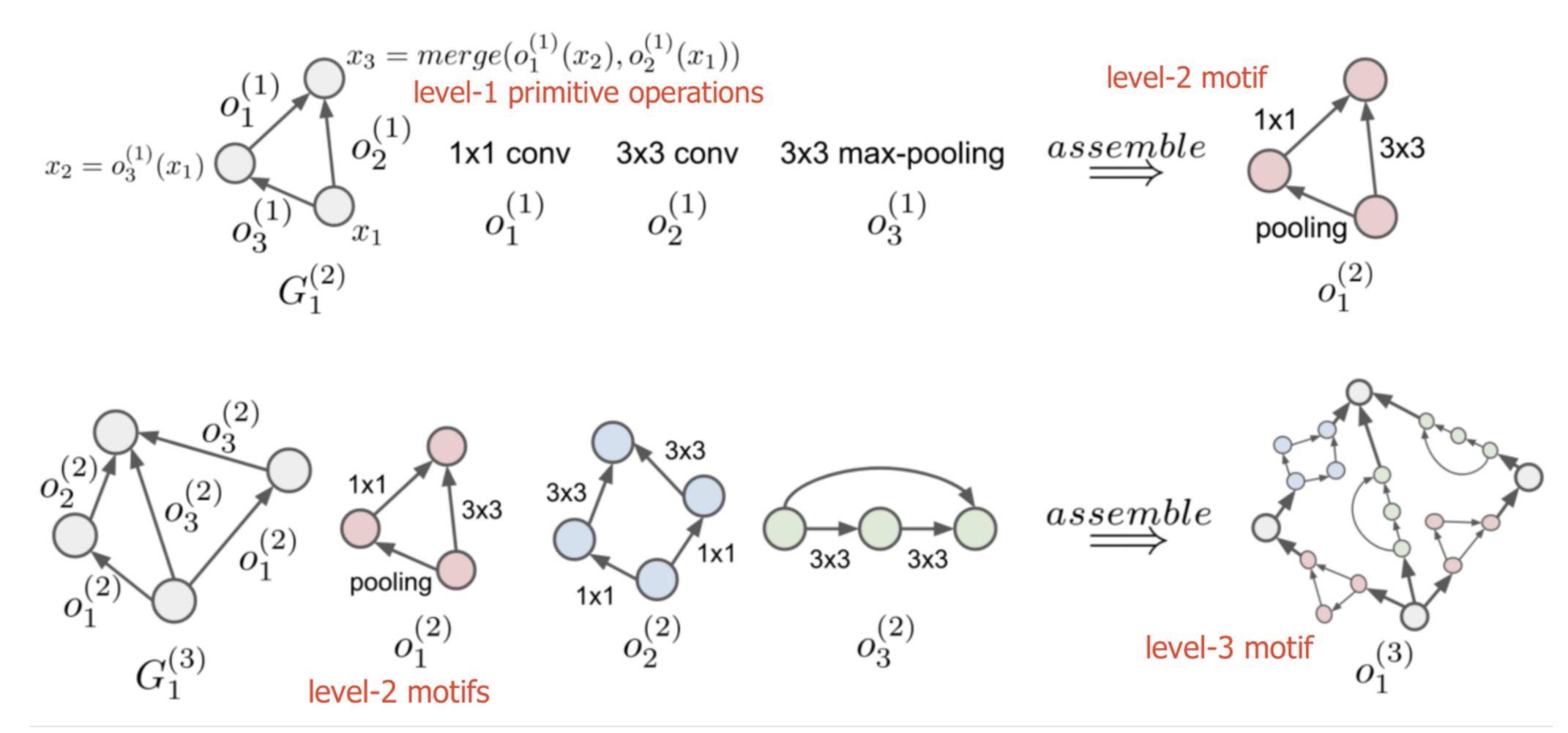
In fact, we can only change the number of layers in many cases, with a fixed hierarchy.



There are several approaches that try to step outside this boundary.

(but they are not as popular as feedforward-like ones, as far as I know)

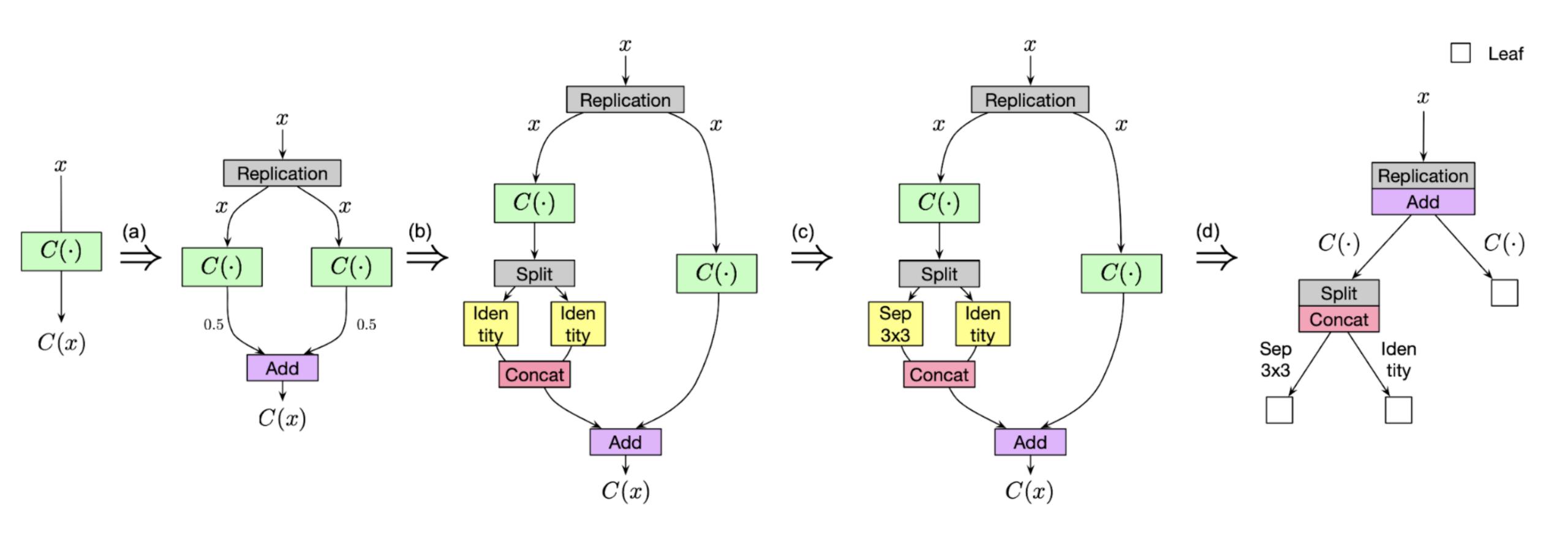
Example. Liu et al. (2018) proposes Hierarchical NAS, which uses *grαph motifs* as a building block.



There are several approaches that try to step outside this boundary.

(but they are not as popular as feedforward-like ones, as far as I know)

Example. Cai et al. (2018) proposes to use tree-like branching process.



Next Up. Search strategies
Performance estimation strategies
Recent papers (transformers?)