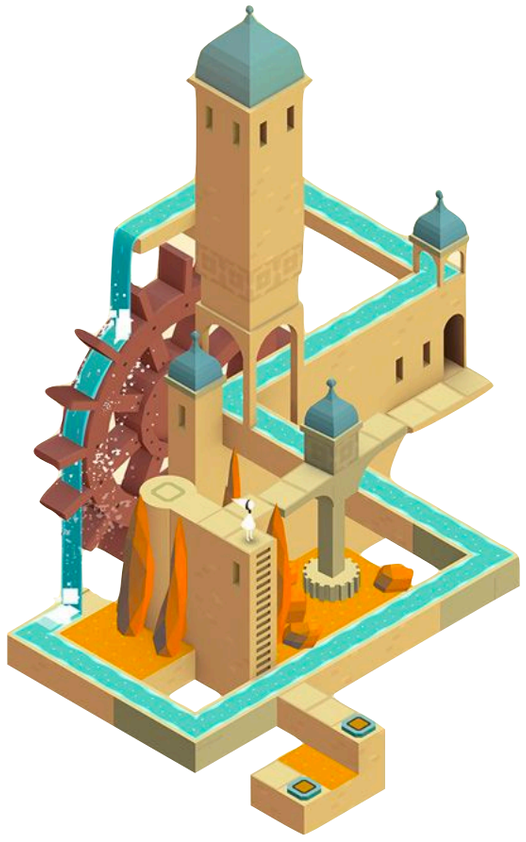
Advanced Course on Data Science & Machine Learning
Siena, 2019



Automatic Machine Learning & Meta-Learning

part 3

Joaquin Vanschoren

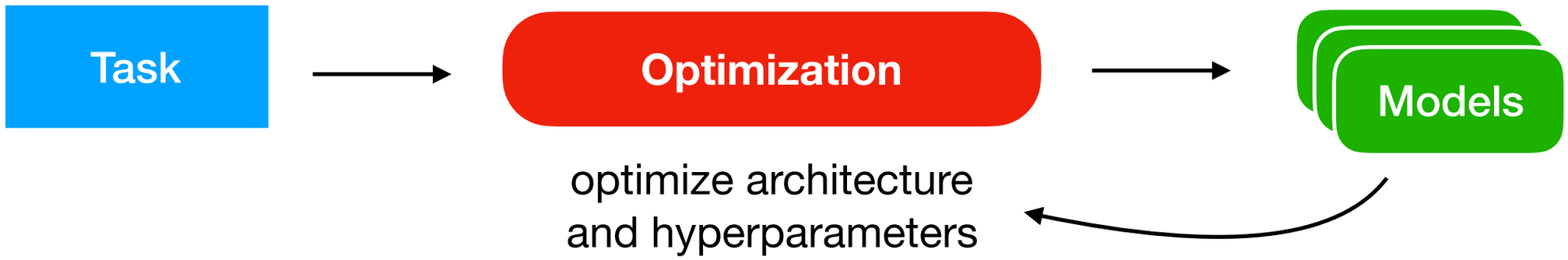
Eindhoven University of Technology

j.vanschoren@tue.nl @joavanschoren http://bit.ly/openml

slides!

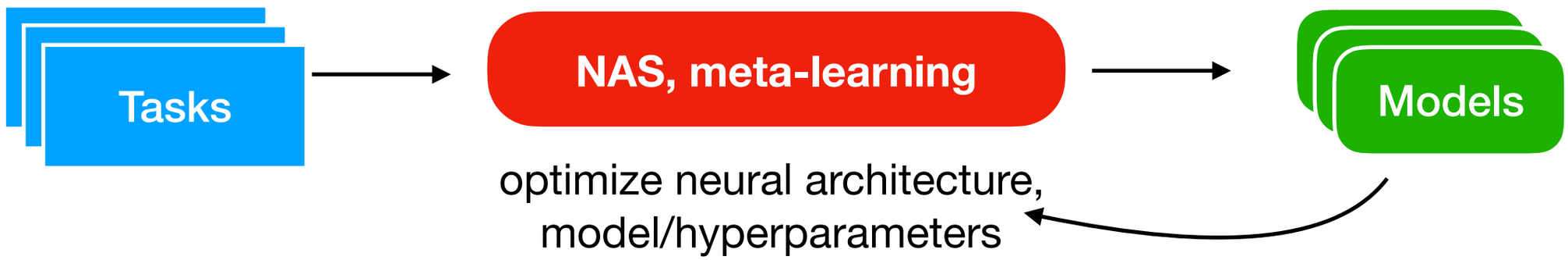
Overview

part 1 AutoML introduction, promising optimization techniques



part 2 Meta-learning

part 3 Neural architecture search, meta-learning on neural nets



Overview

part 3 Neural architecture search, meta-learning on neural nets

1. Neural Architecture Search space
2. Neural Architecture optimization
3. (Neural) Meta-Learning

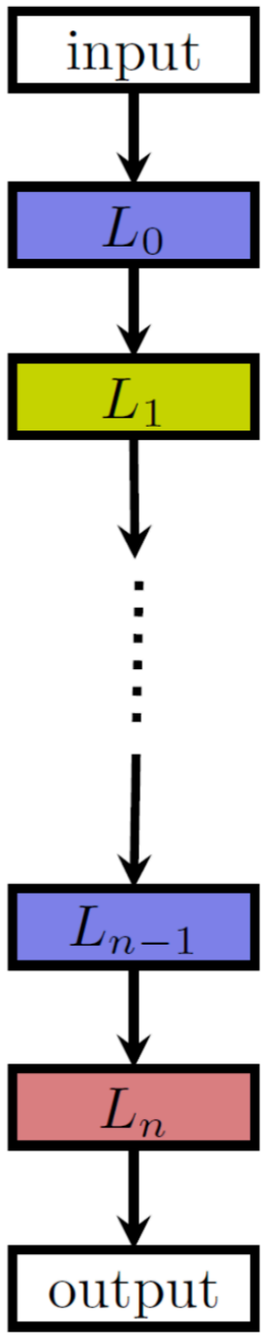
Neural Architecture Search space

Sequential (chain)

Choose:

- number of layers
- type of layers
  - dense
  - convolutional
  - max-pooling
  - …
- hyperparameters of layers

+ easier to search
- sometimes too simple

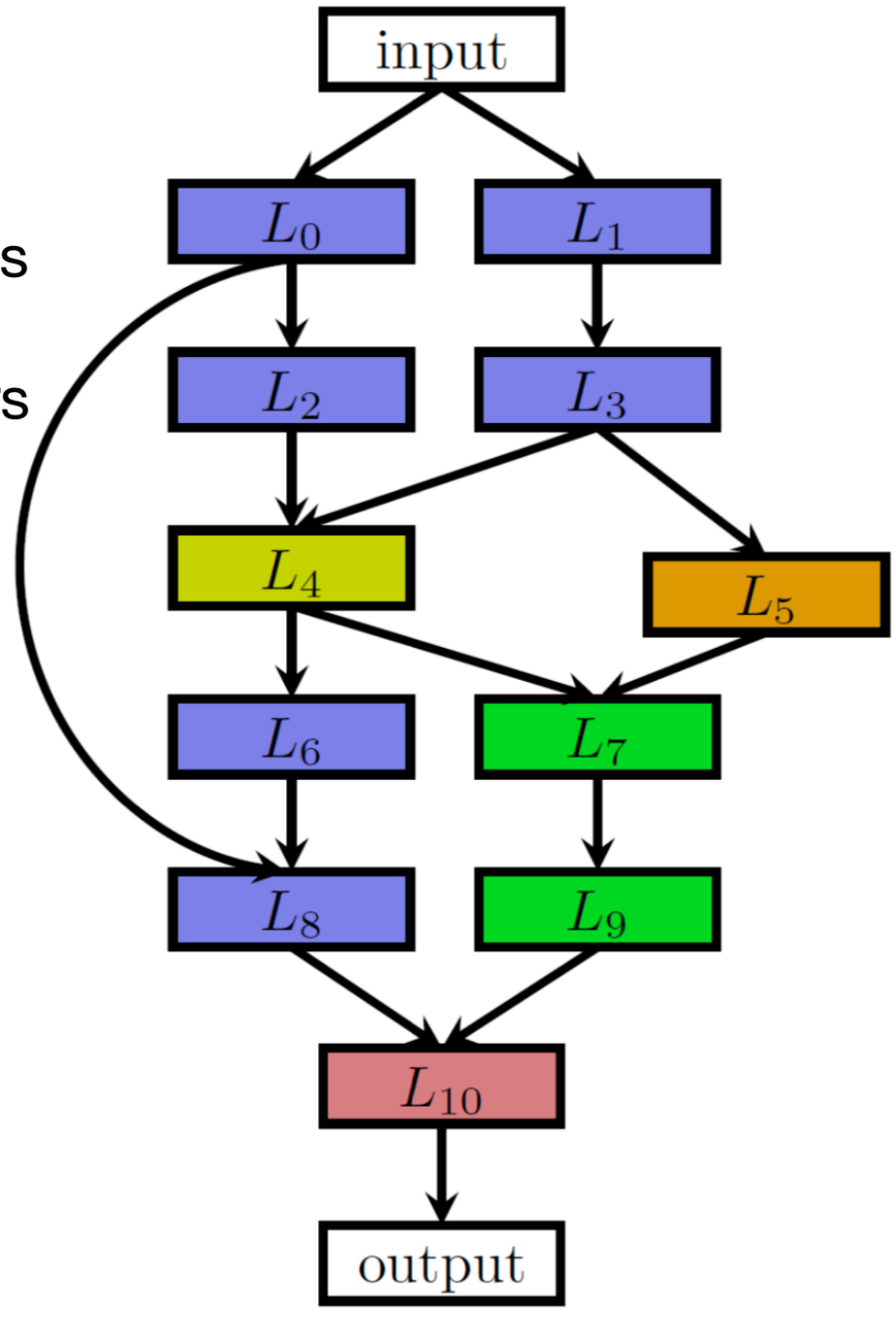


Arbitrary graph

Choose:

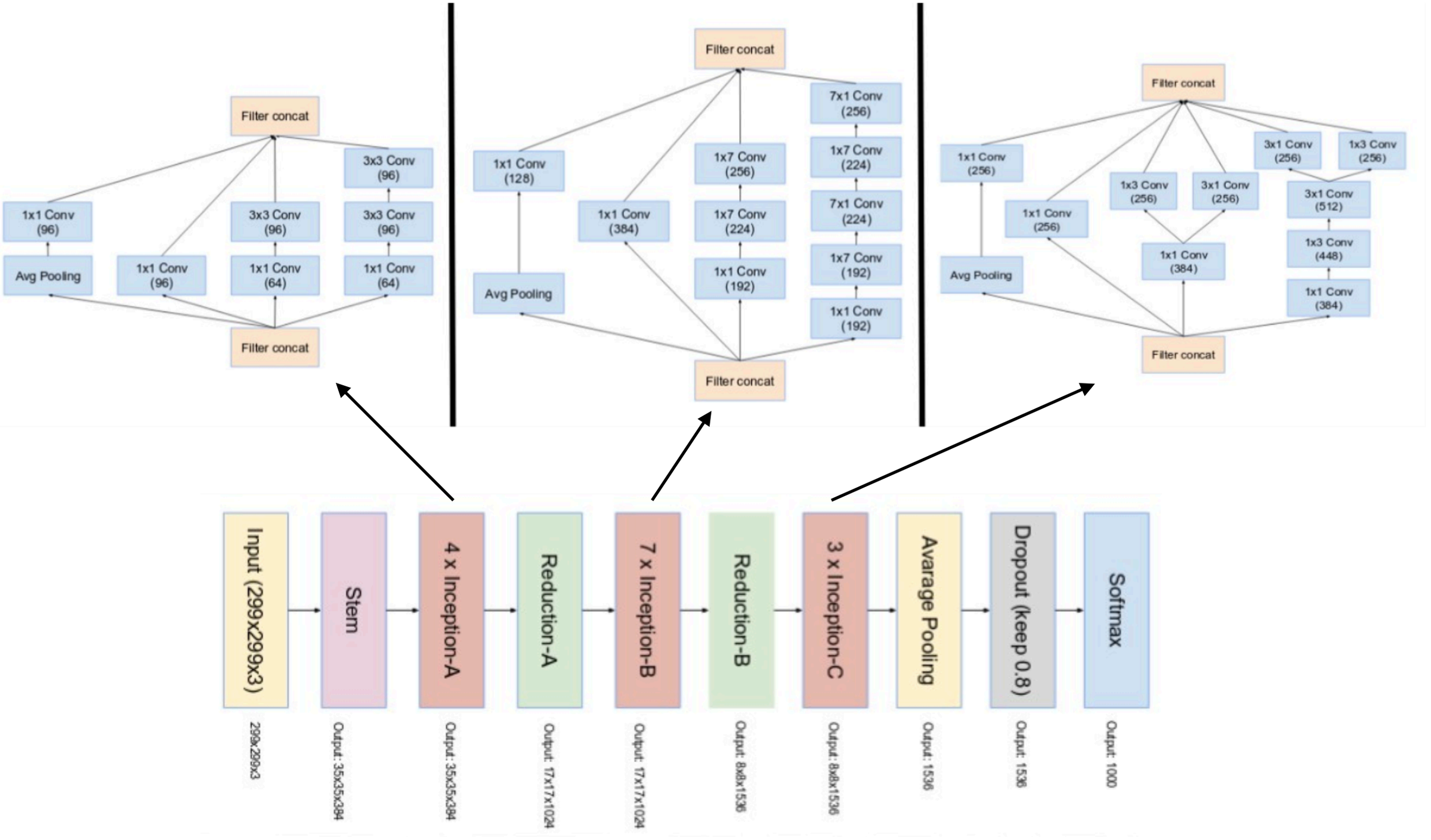
- branching
- joins
- skip connections
- types of layers
- hyperparameters of layers

+ more flexible
- much harder to search



Neural Architecture Search space

Observation: successful deep networks have repeated motifs (cells)
e.g. Inception v4:

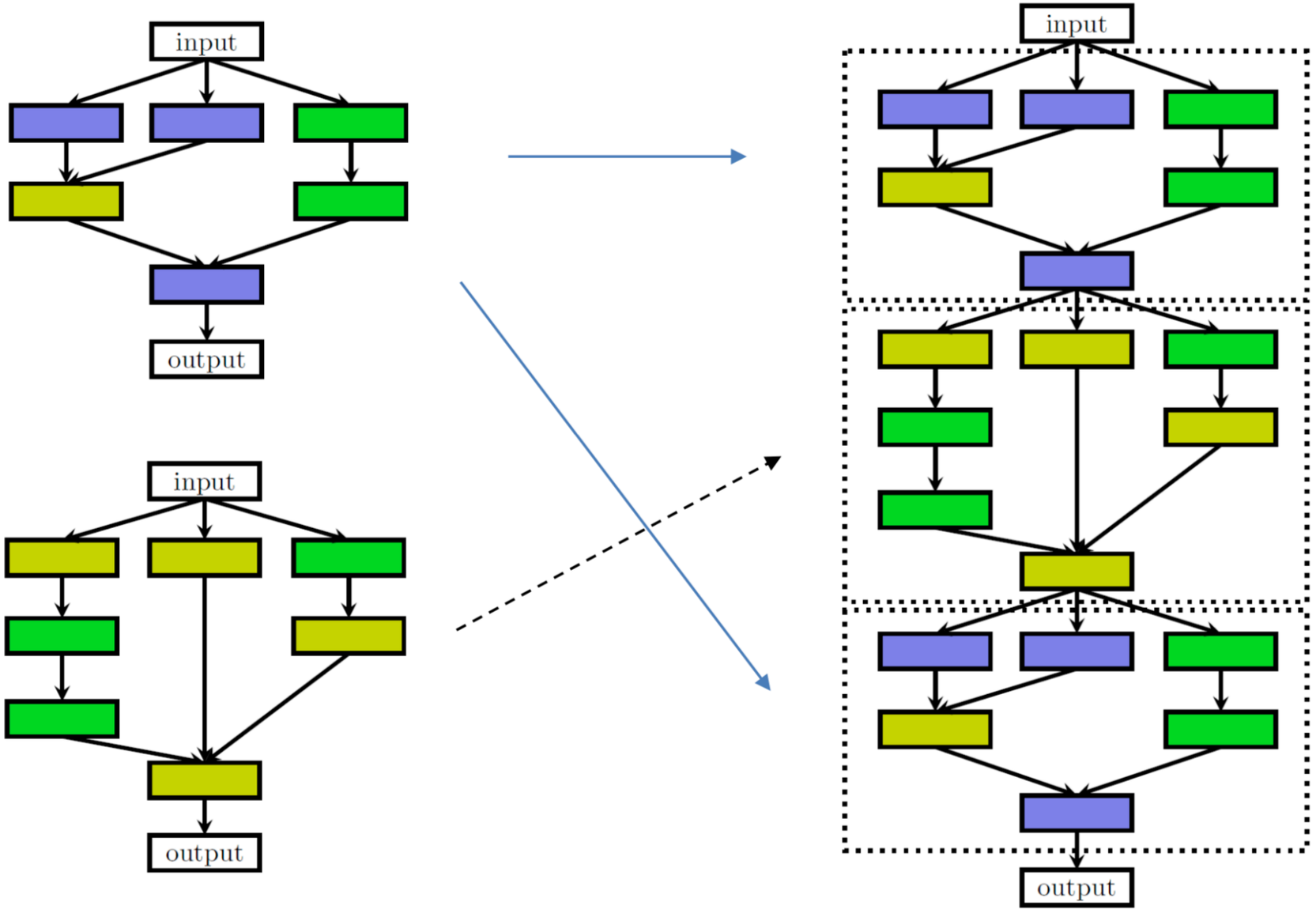


Zoph et al 2018

Cell search space

- parameterize building blocks *(cells)*
  - *e.g. regular cell + resolution reduction cell*

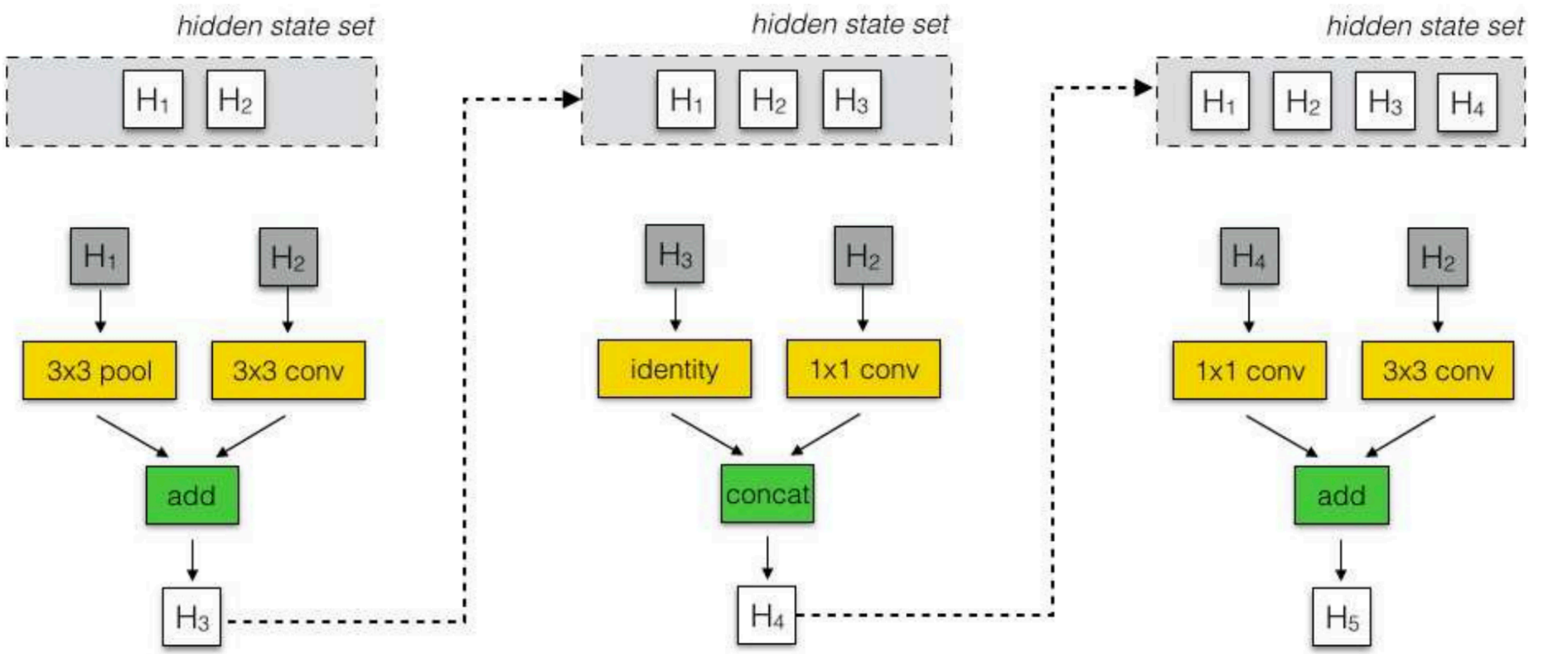
- stack cells together in macro-architecture
  - usually a chain
  - can be manual or learned



+ smaller search space
+ cells can be learned on a small dataset & transferred to a larger dataset
- you can't learn entirely new architectures

Within-cell search space

- Different *strategies* to construct cell, leading to different parameterizations
- Can be parameterized as set of categorical hyperparameters:
  - Which existing layer (hidden state, e.g. cell input) H_i to build on
  - Which operation (e.g. 3x3conv) to perform on H_i
  - How to combine into new hidden state
  - Iterate over *B* phases (blocks)



[1] Bergstra et al. 2013

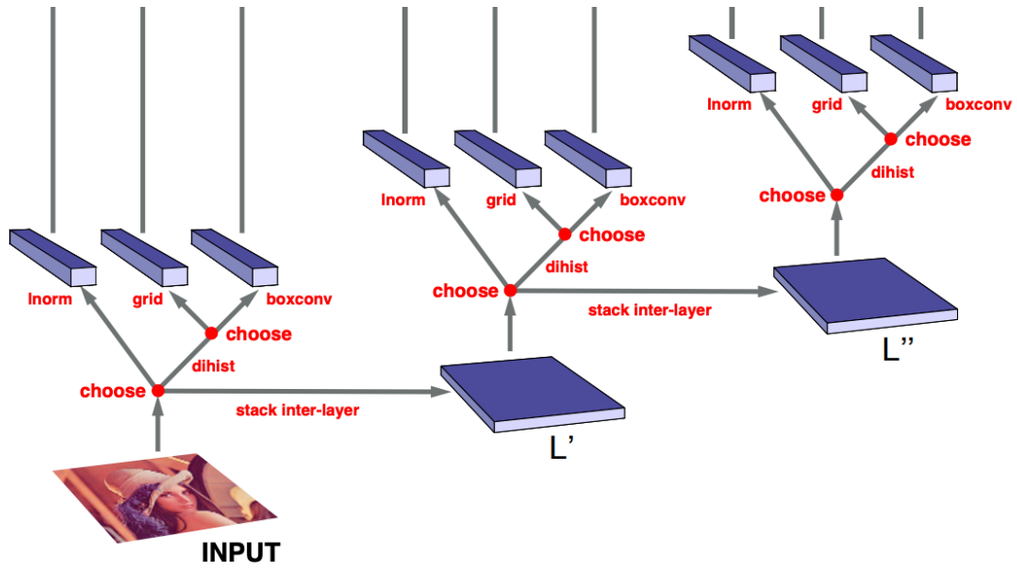
[2] Swersky et al 2013

[3] Kandasamy et al. 2018

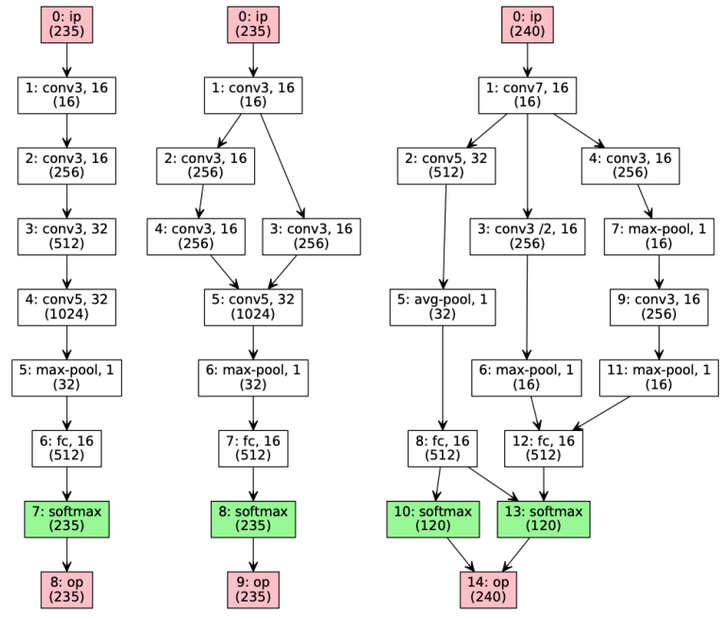
Neural architecture optimization

Standard hyperparameter optimization techniques

- Image classification pipelines[1]
  - 238 hyperparameters, tuned with TPE



- Kernels to optimize neural nets with GP-based Bayesian optimization
  - ArcNet[2]: DNNs, 23 hyperparameters, 6 kernels
  - NASBOT[3]: DNNs and CNNs



[1] Mendoza et al. 2016

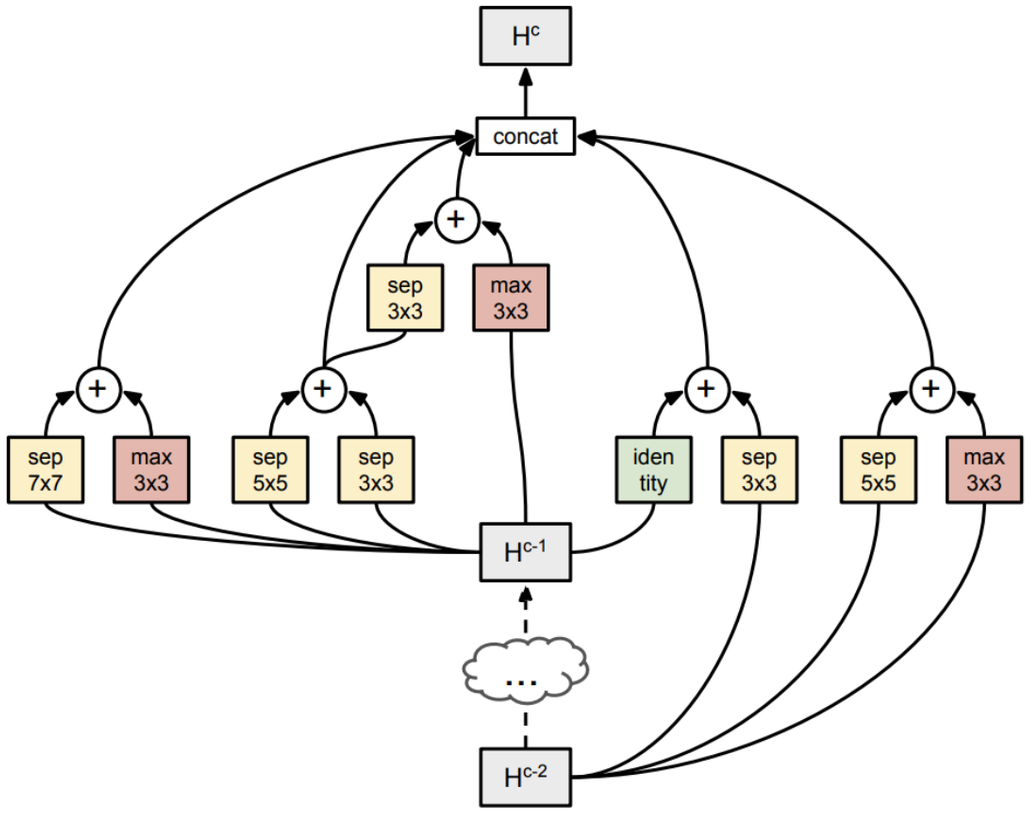
[2] Zela et al. 2018

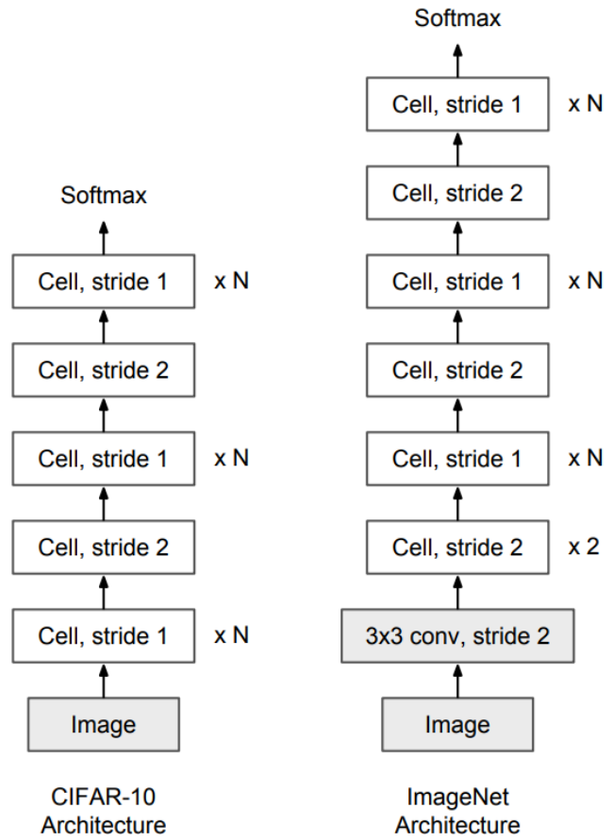
[3] Liu et al. 2018

Neural architecture optimization

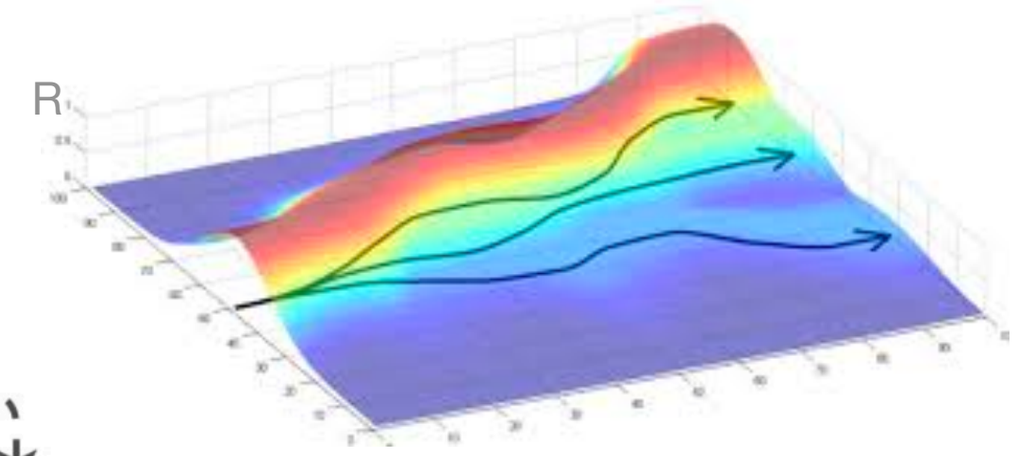
Standard hyperparameter optimization techniques

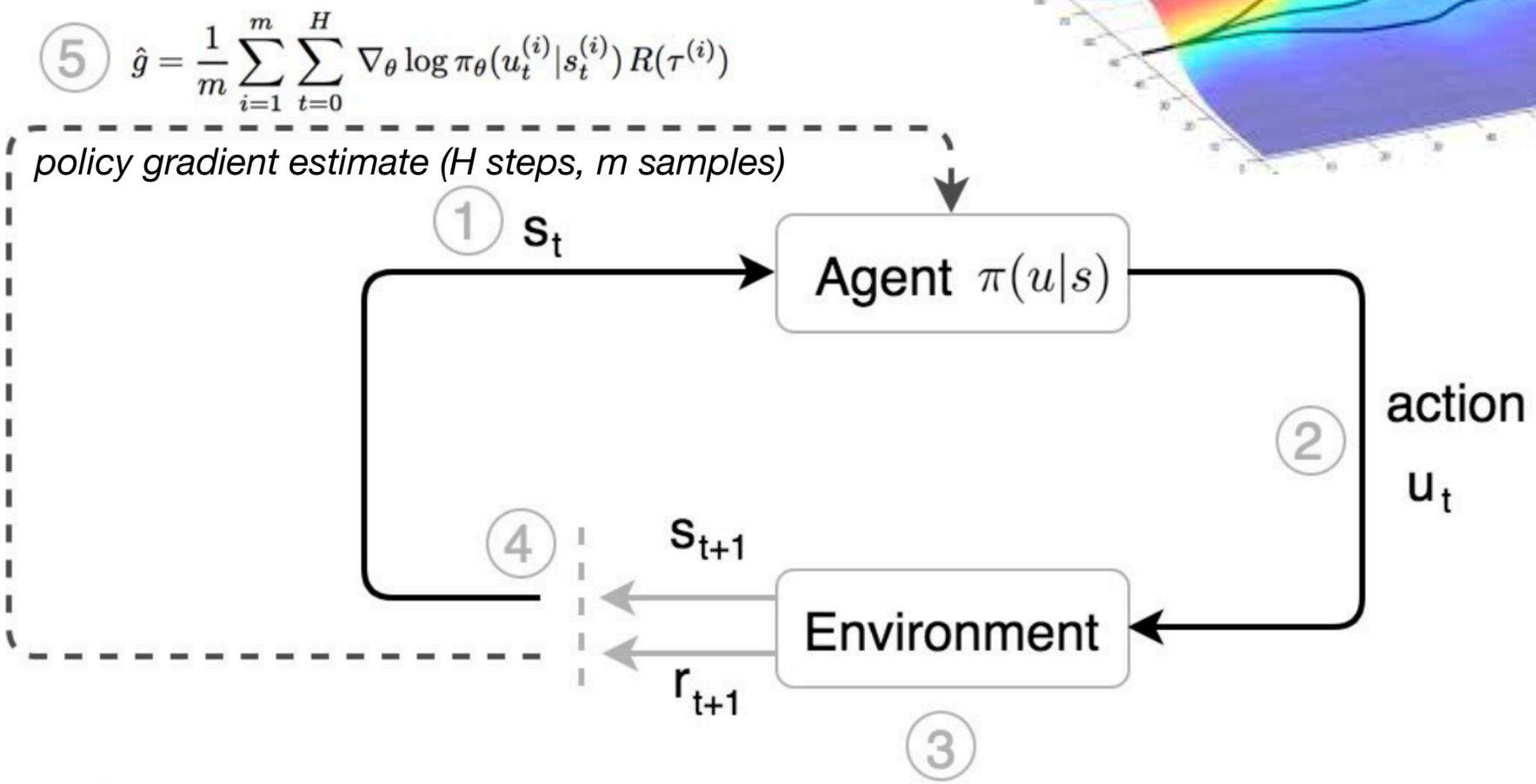
- AutoNet [1] : DNNs, 63 hyperparameters, tuned with SMAC
- Joint NAS + HPO [2]: ResNets, tuned with BO-HB
- PNAS (Progressive NAS) [3]
  - Cell search space, optimized with SMAC, HPO afterwards
  - SotA on ImageNet, CIFAR





Deep RL recap





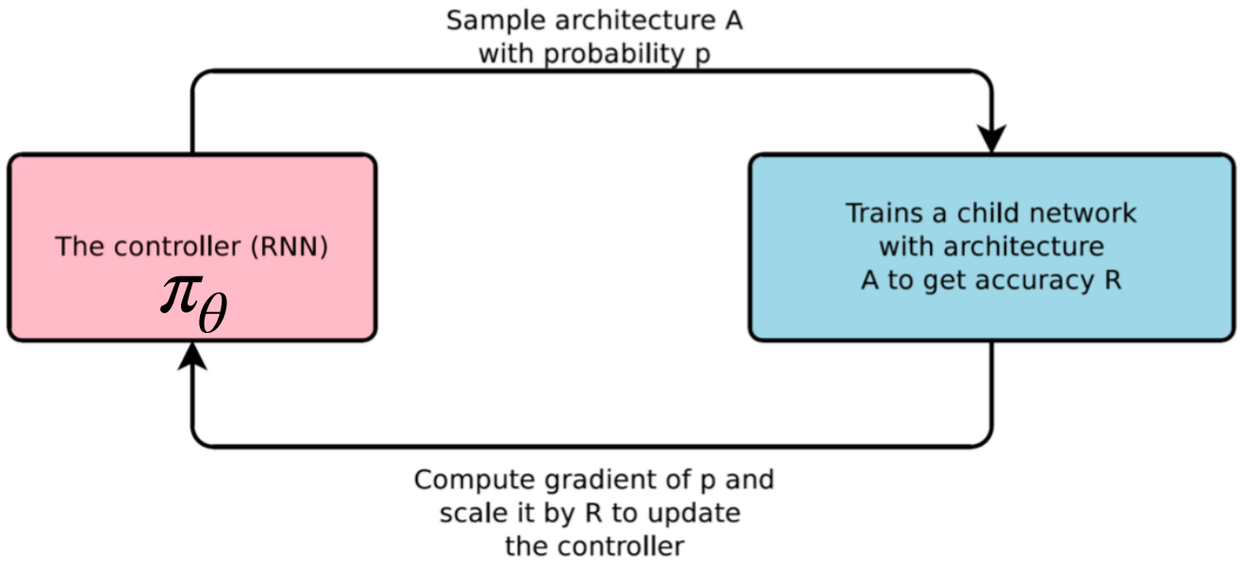
1. Observe state
2. Take action *u* based on policy π_θ (θ are weights in an RNN)
3. New state is formed
4. Take further actions based on new state
5. After trajectory τ of motions, adjust policy based on total reward R(τ)

Zoph & Le 2017

NAS with Reinforcement learning

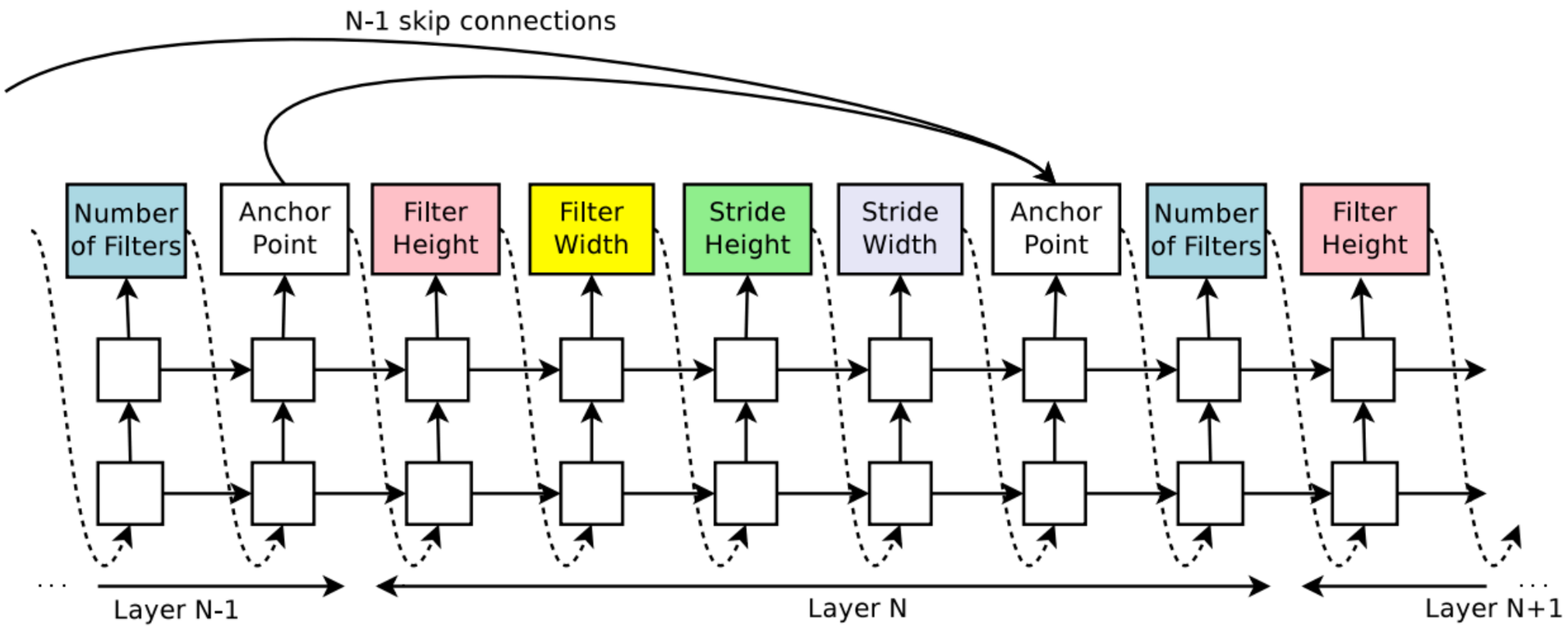
RNN policy network:

- generate architecture step by step
- evaluate to get reward
- update with policy gradient



2-layer LSTM (REINFORCE), chains of convolutional layers

- State of the art on CIFAR-10, Penn Treebank
- 800 GPUs for 3-4 weeks, 12800 architectures

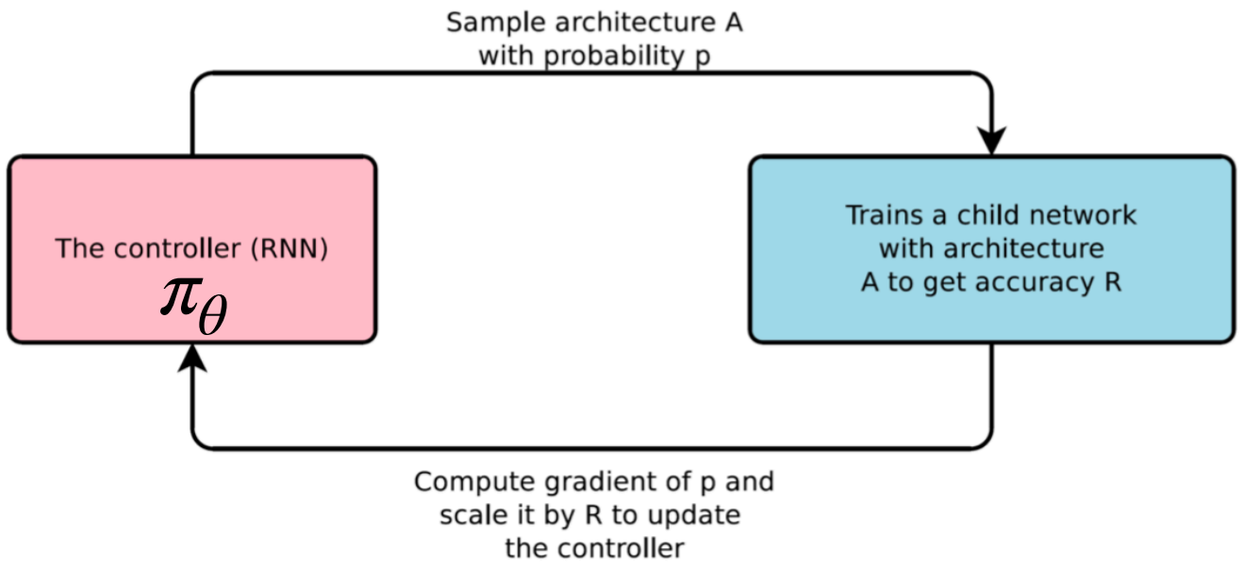


Zoph et al 2018

NAS with Reinforcement learning

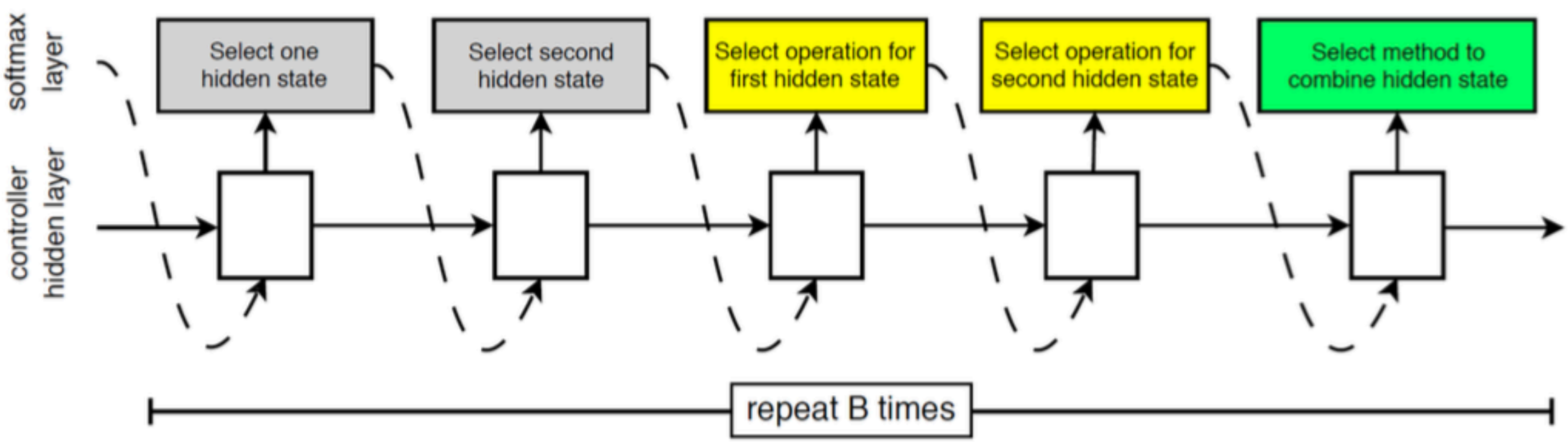
RNN policy network:

- generate architecture step by step
- evaluate to get reward
- update with policy gradient



1-layer LSTM (PPO), cell space search

- State of the art on ImageNet
- 450 GPUs, 20000 architectures

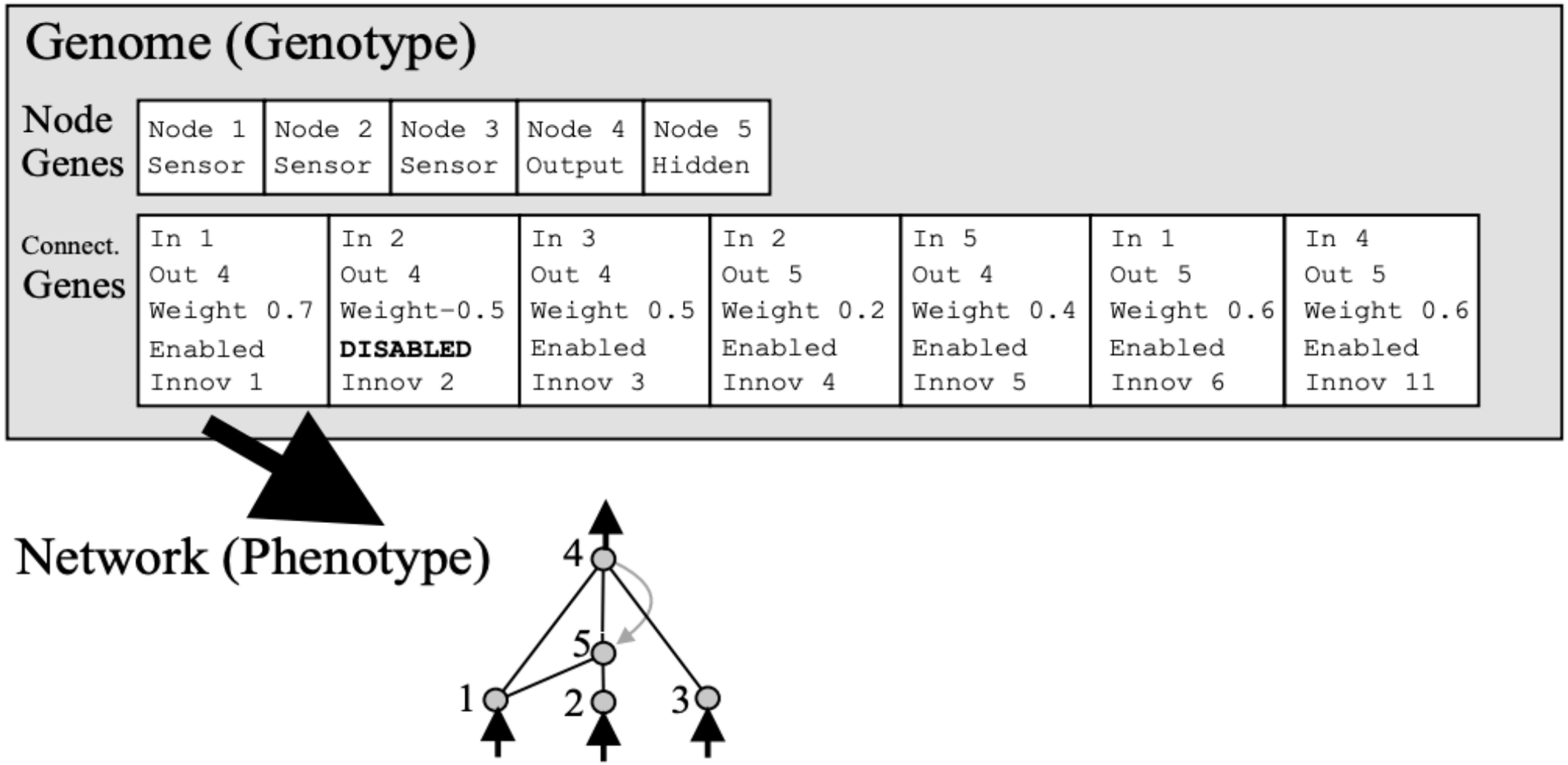


Angeline et al 1994, *Stanley and Miikkulainen 2002*

Neuroevolution

Earlier solutions tried to:

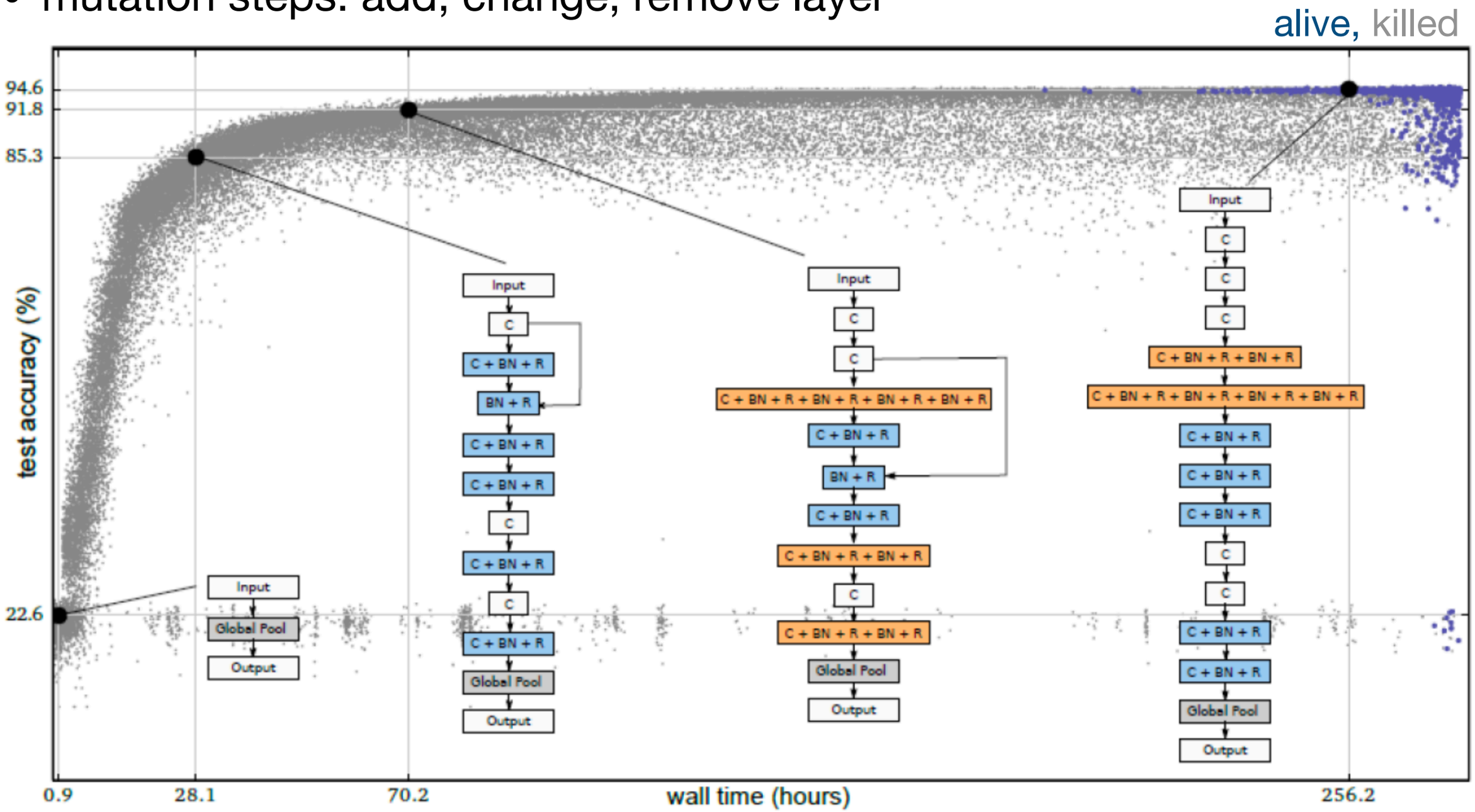
- Optimize both the configuration and the weights simultaneously with genetic algorithms
- Optimize individual nodes and connections
- Doesn't scale to deep networks



Neuroevolution

Better:

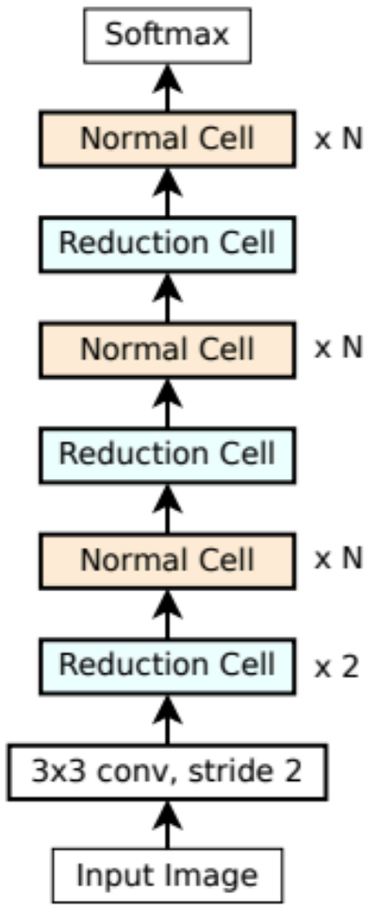
- learn the architecture and configuration with evolutionary techniques
- train the network with SGD
- mutation steps: add, change, remove layer

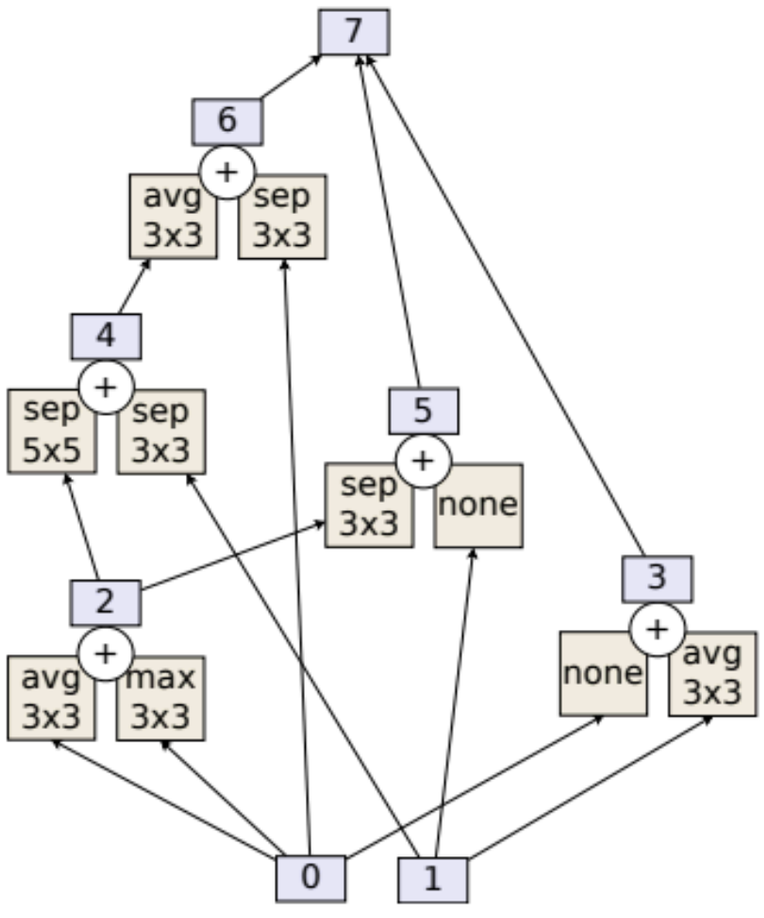


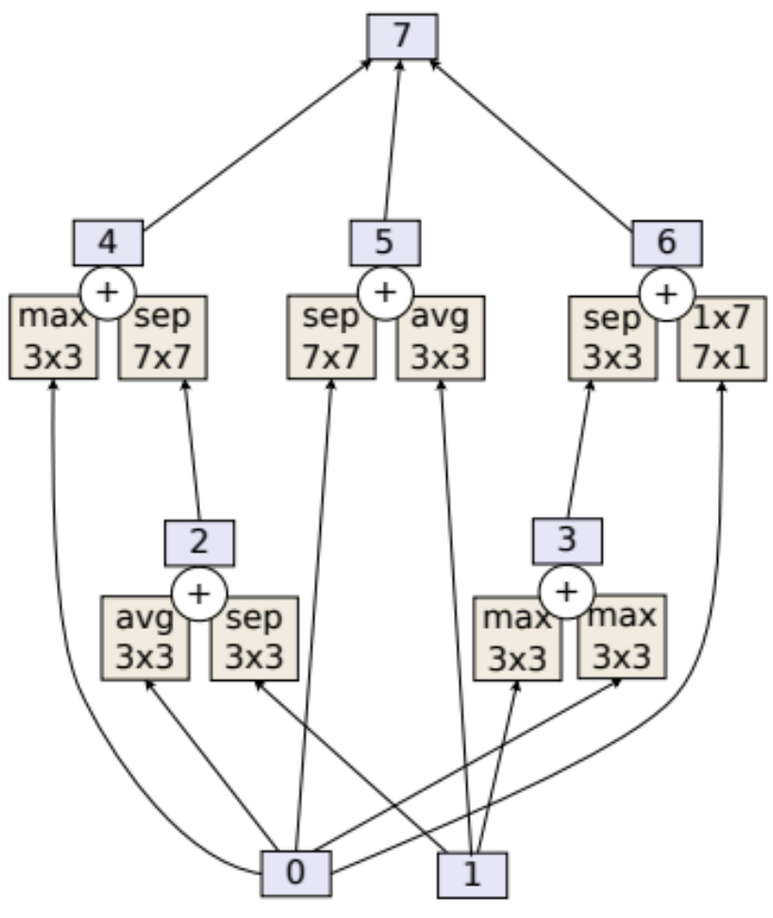
Neuroevolution

AmoebaNet: State of the art on ImageNet, CIFAR-10

- Cell search space, aging evolution (kill oldest networks)





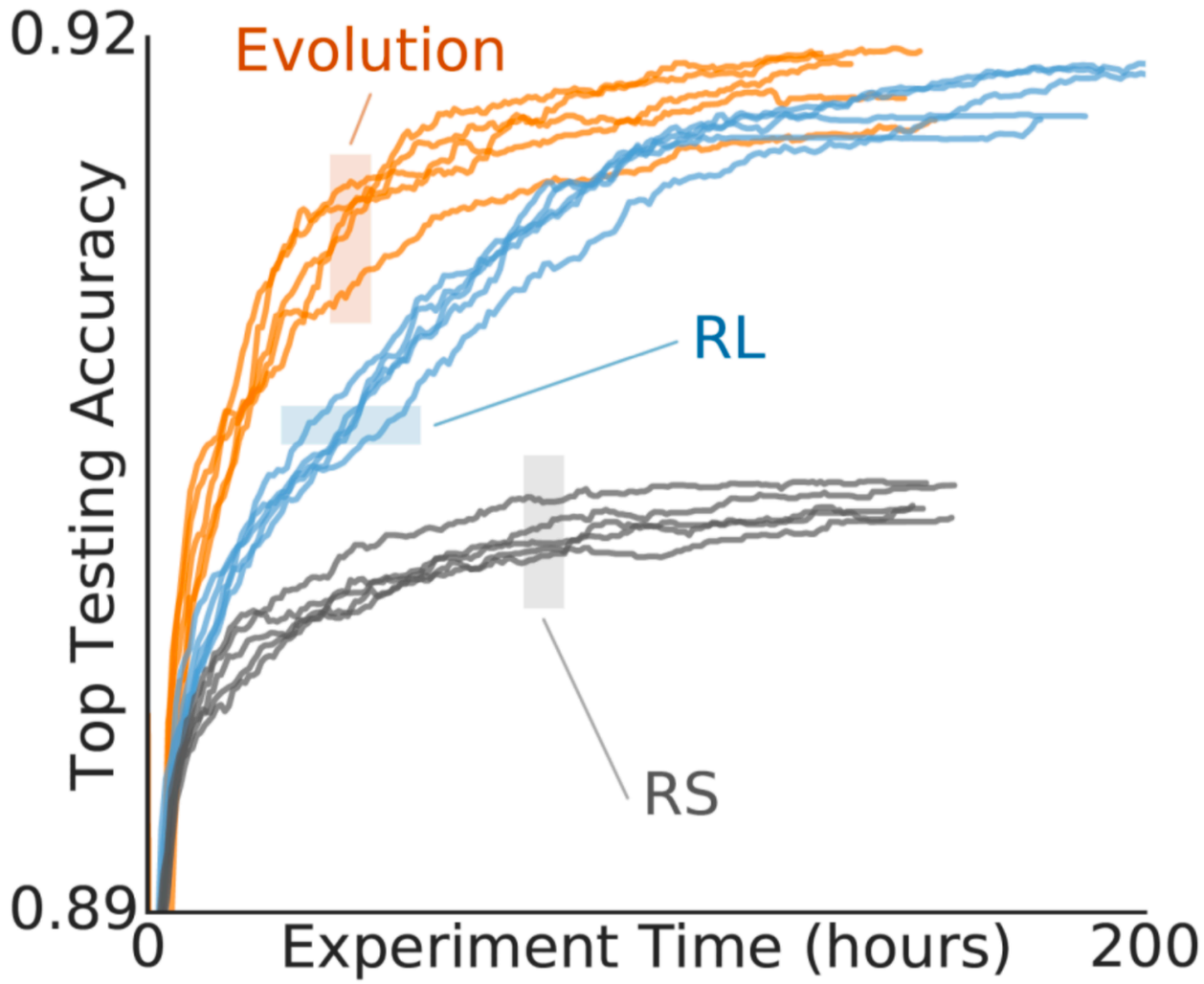


Real et al 2019

Neuroevolution

AmoebaNet: State of the art on ImageNet, CIFAR-10

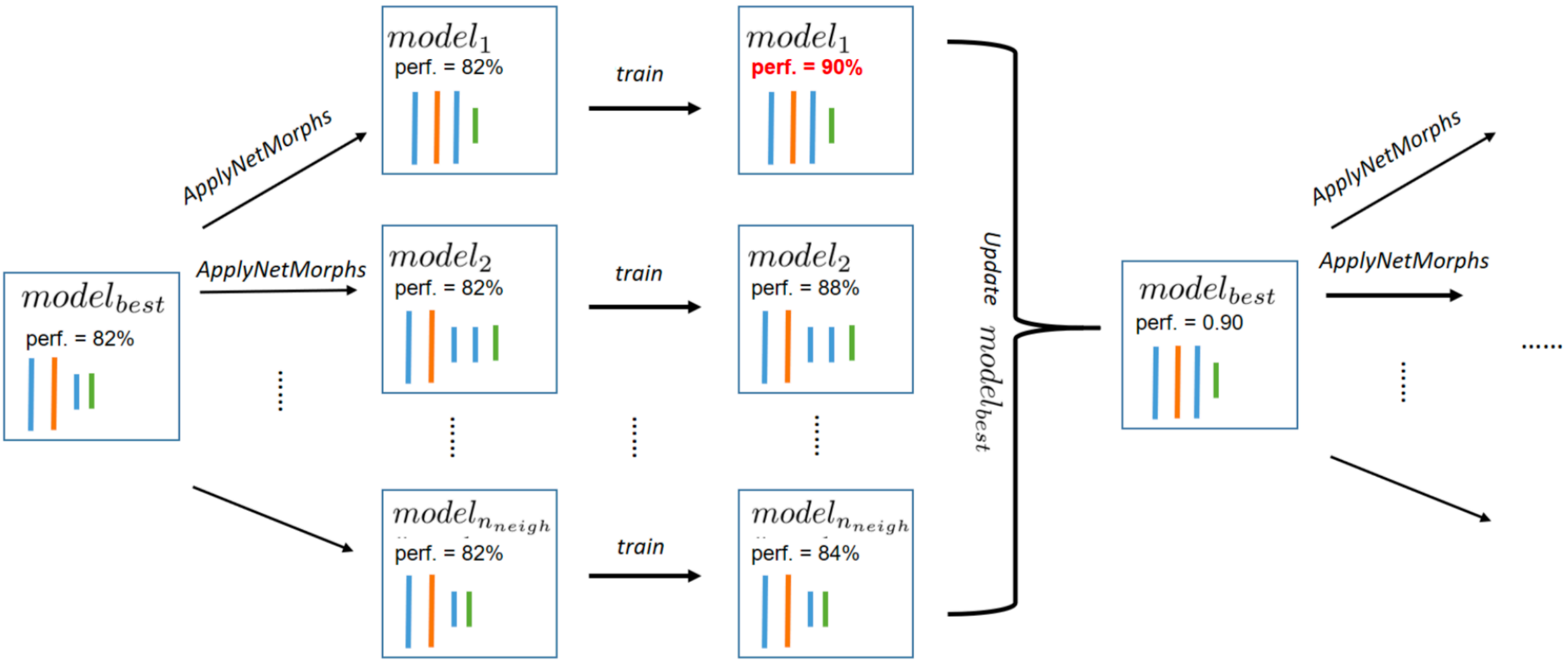
- Cell search space, aging evolution (kill oldest networks)
- More efficient than reinforcement learning



[Chen et al. 2016](), [Wei et al. 2016](), [Cai et al. 2017]()
[Cai et al. 2018](), [Elsken et al. 2017](), [Cortes et al. 2017](), [Cai et al. 2018]()

Network morphisms

- Change architecture, but not modelled function
- Non-black box, allows much more efficient architecture search



[1] Saxena & Verbeek, 2016

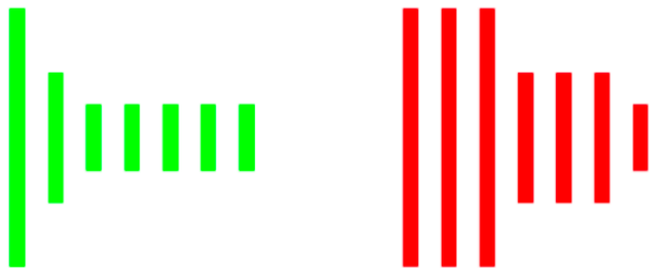
[2] Bender et al. 2018

[3] Pham et al. 2018

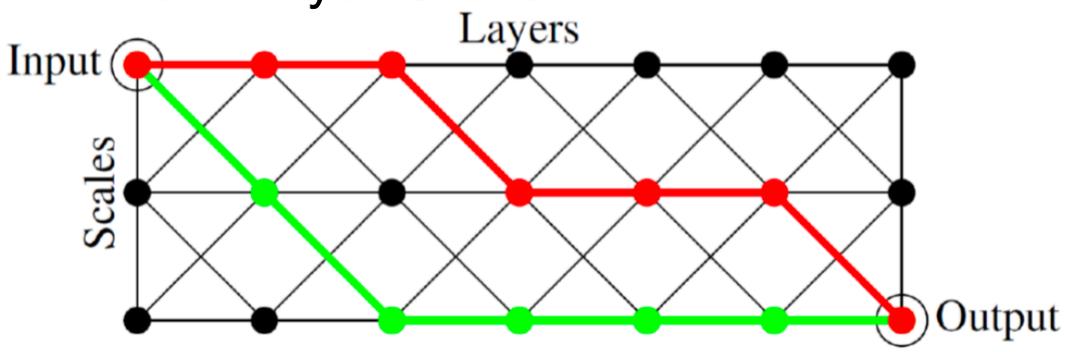
[4] Brock et al. 2017

Weight sharing

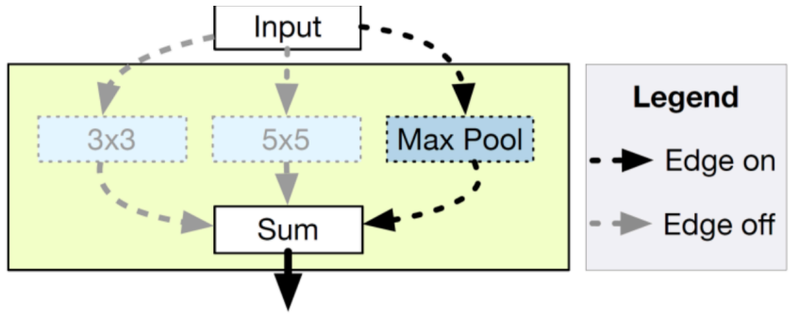
- One-shot models (convolutional neural fabric) [1]
  - Search space: ConvNet = path though *fabric* with shared weights
  - Train ensemble of all of them



For 7-layer CNNs:



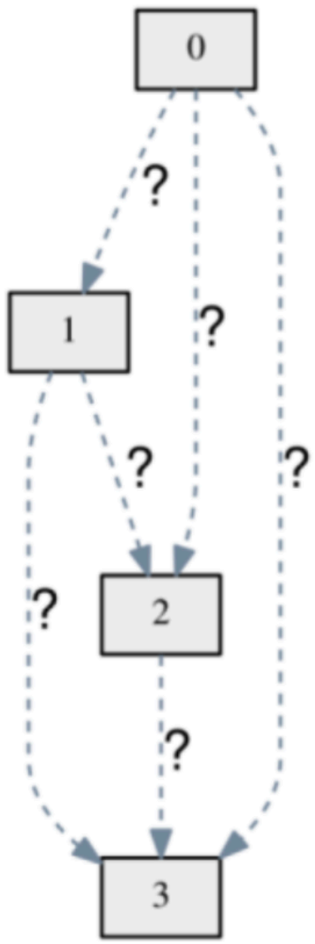
- *Path dropout* [2]
  - ensure that individual paths do well



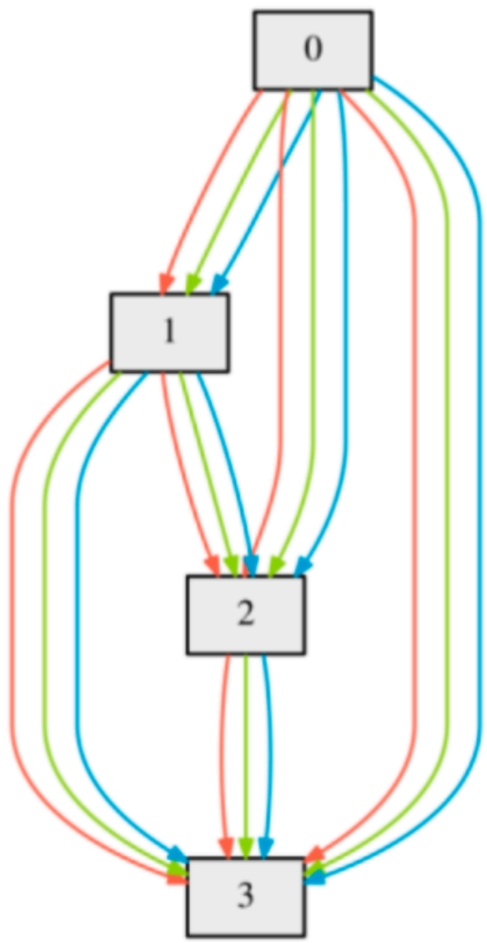
- *ENAS* [3]
  - use RL to sample paths from one-shot model, train weights
  - other paths inherit these weights
- *SMASH* [4]
  - Shared hypernetwork that predicts weights given architecture

DARTS: Differentiable NAS

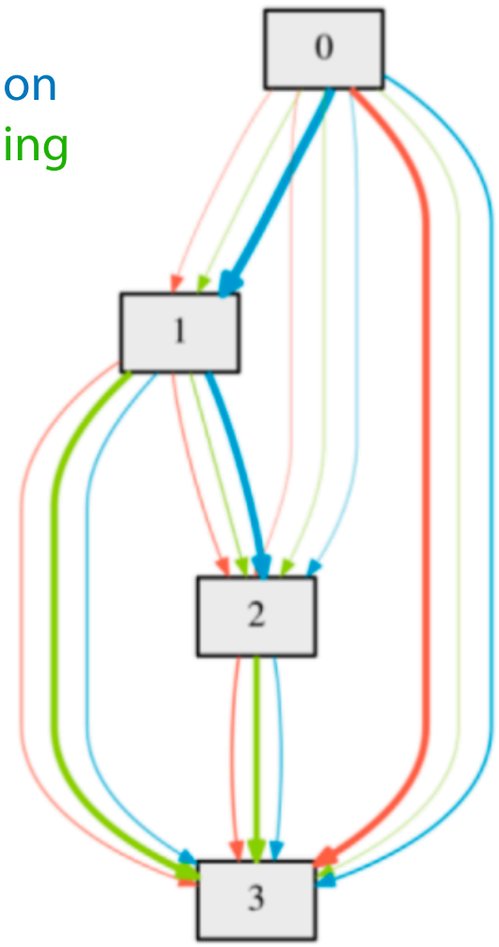
- Fixed (one-shot) structure, learn which operators to use
- Give all operators a weight α_i
- Optimize α_i and model weights ω_j using bilevel programming



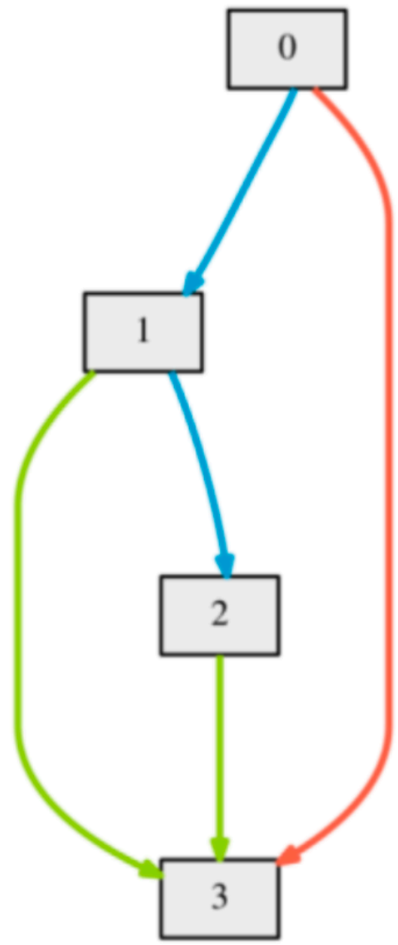
One-shot model



operator weights α_i



interleaved optimization of α_i and ω_j with SGD



argmax α_i

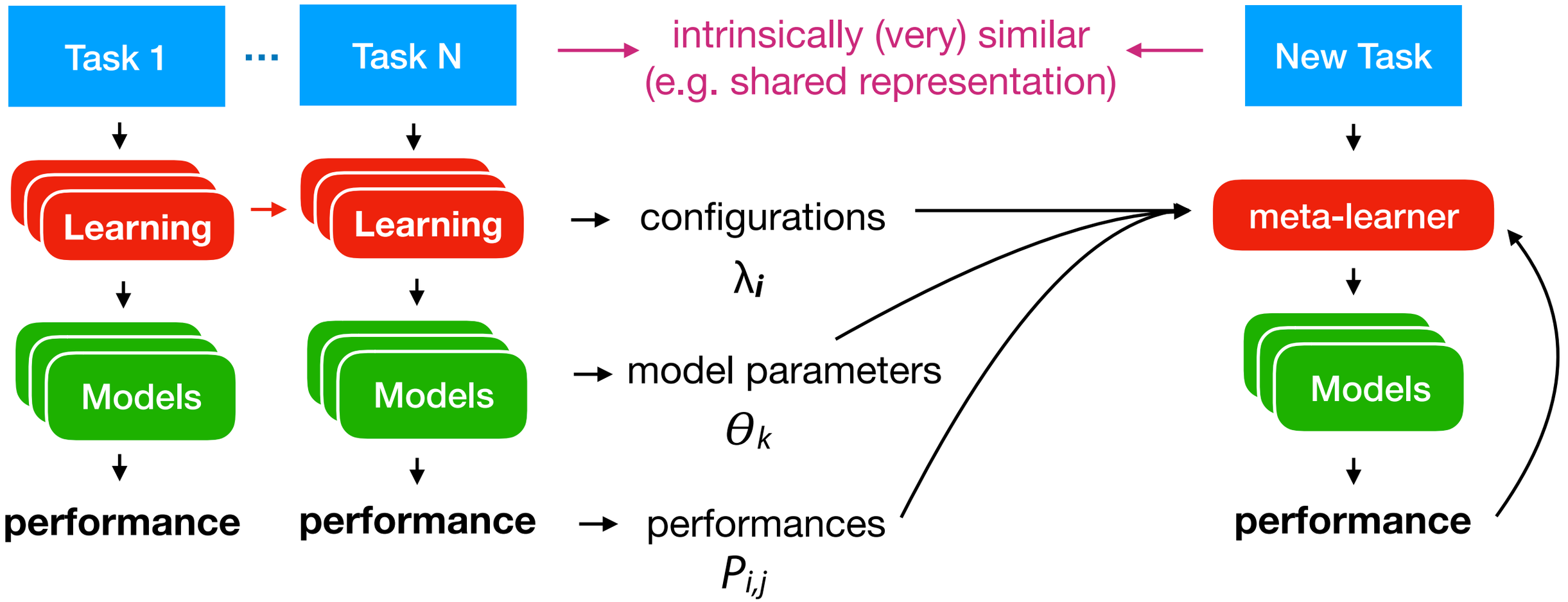
DARTS: Differentiable NAS

- Lots of further refinements
  - SNAS *[Xie et al 2019]*
    - Use Gumbel softmax (differentiable) on α_i
  - Proxyless NAS *[Cai et al 2019]*
    - Memory-efficient DARTS
      - trains sparse architectures only
  - …

Learning to learn from previous *models*

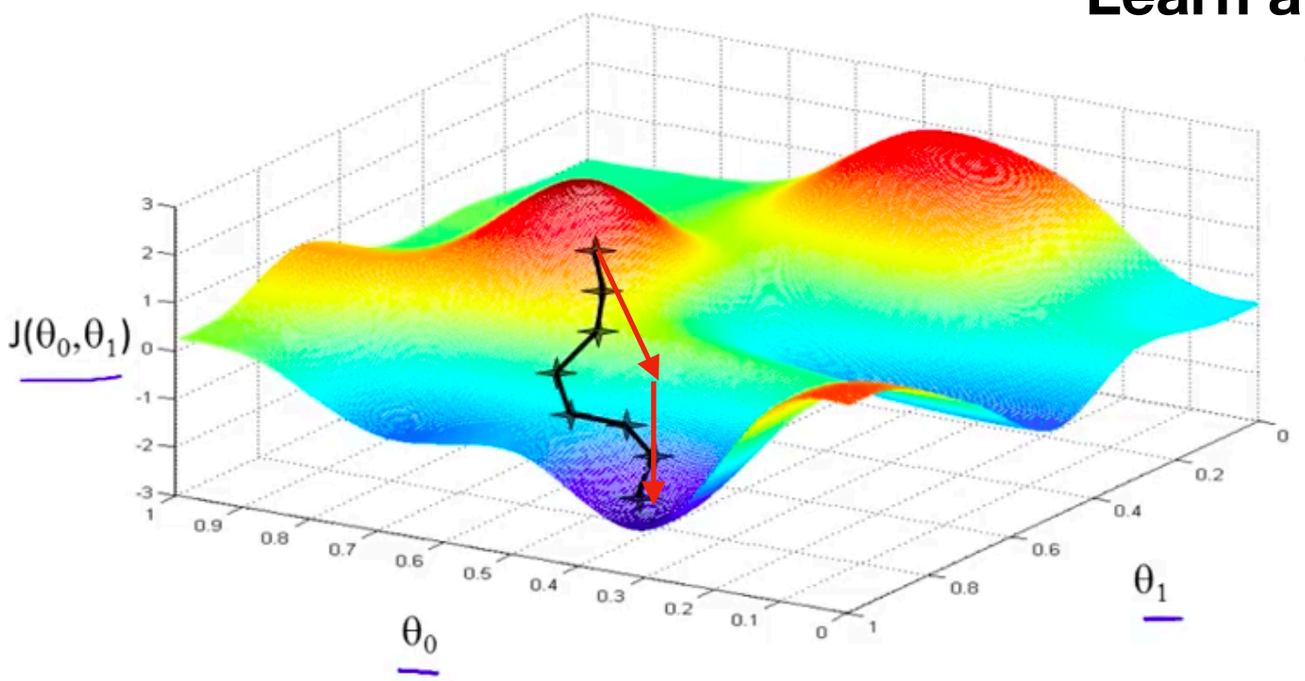
For models trained on intrinsically similar tasks

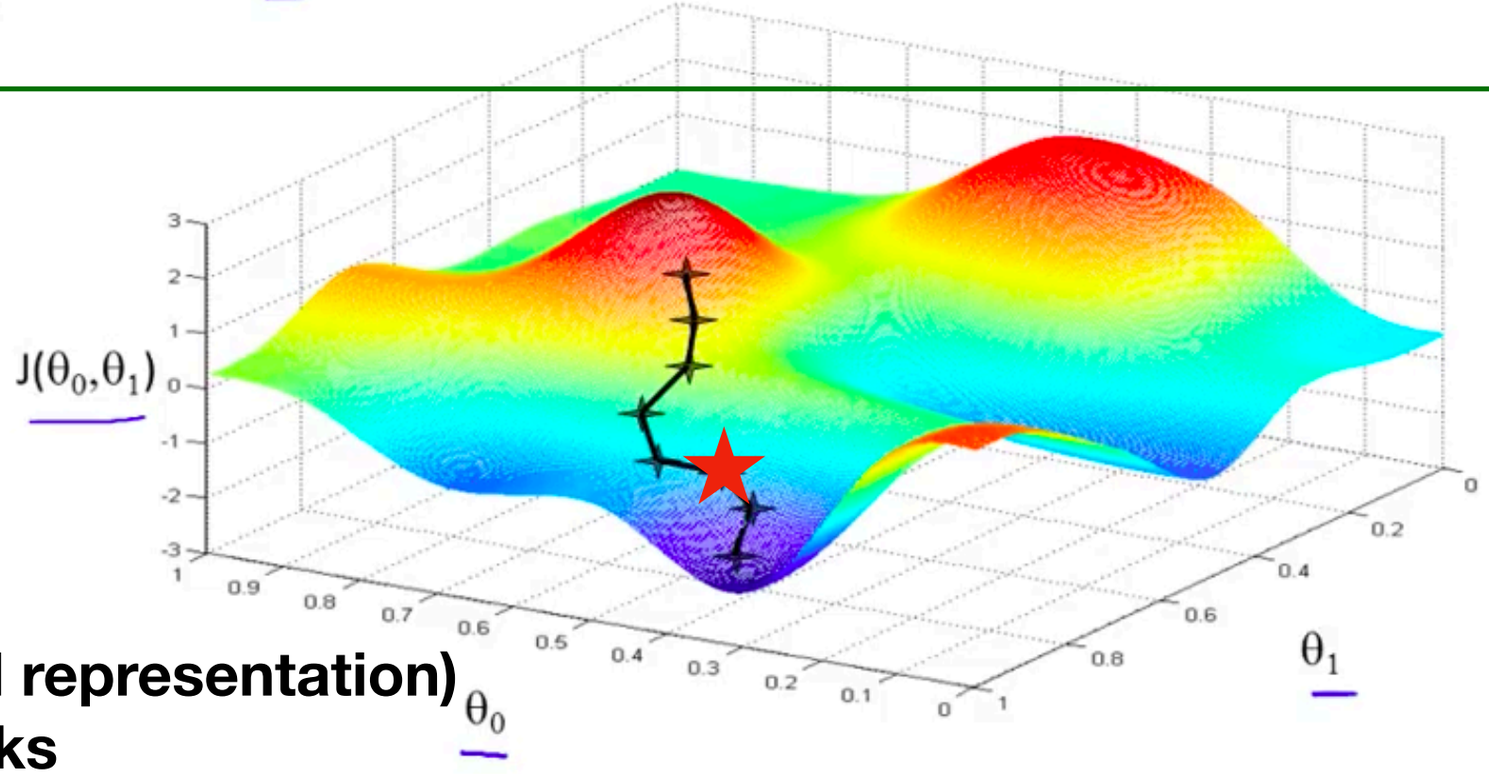
(model parameters, features,…)



Learning to learn

Learn a better gradient update rule for a group of tasks





Learn a better initialization (and representation) for a group of tasks

[1] Bengio et al. 1995

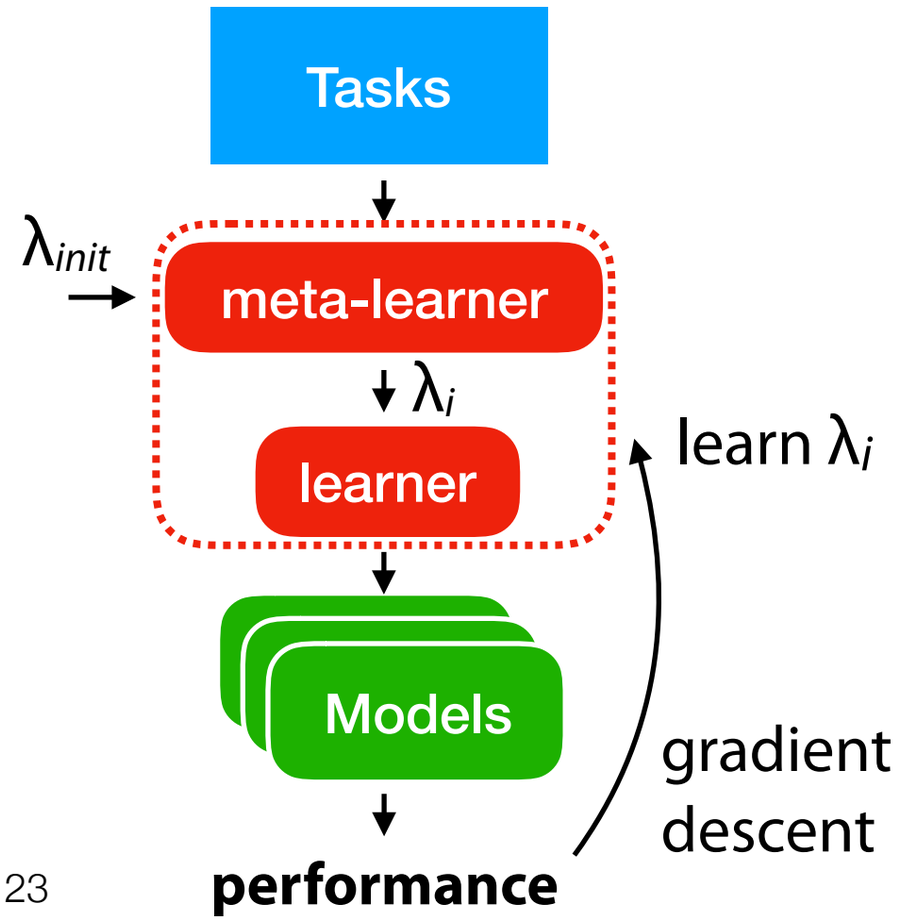
[2] Runarsson and Jonsson 2000

Learning to learn by gradient descent

- Our brains *probably* don't do backprop, replace it with:

$$\Delta w_{ij} = -\eta \frac{\partial E_p}{\partial w_{ij}}$$

  - Simple *parametric* (bio-inspired) rule to update weights [1]
  - Single-layer neural network to learn weight updates [2]
- Learn parameters across tasks, by gradient descent (meta-gradient)



Bengio et al.

$$\Delta \theta_i = \epsilon \, y_{pre(i)} \, k$$

presynaptic activity

learning rate

reinforcing signal

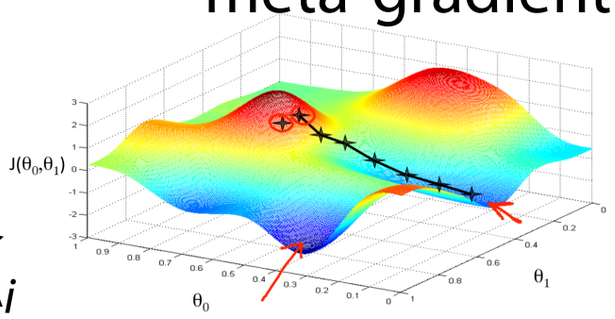
Runarsson and Jonsson

$$\Delta \theta_i = \eta \, (\quad)$$

learning rate

weights λ_i

meta-gradient

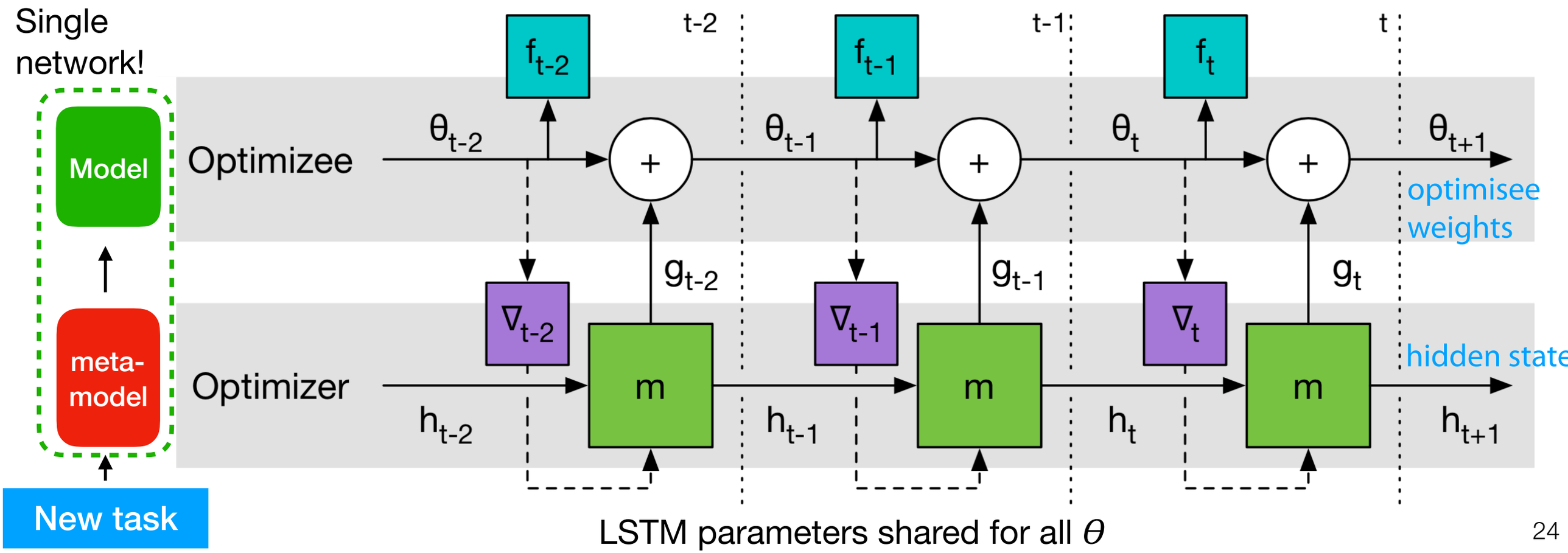


[1] Hochreiter 2001

[2] Andrychowicz et al. 2016

Learning to learn gradient descent by gradient descent

- Replace backprop with a recurrent neural net (LSTM)[1], not so scalable
- Use a coordinatewise LSTM [m] for scalability/flexibility (cfr. ADAM, RMSprop) [2]
  - Optimizee: receives weight update g_t from optimizer
  - Optimizer: receives gradient estimate ∇_t from optimizee
    - Learns how to do gradient descent across tasks



[1] Hochreiter 2001

[2] Andrychowicz et al. 2016

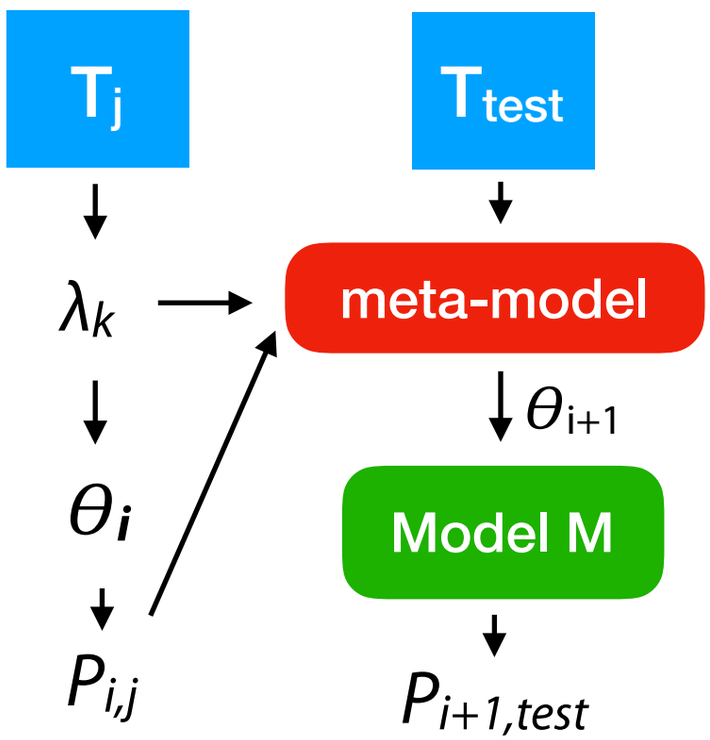
Learning to learn gradient descent by gradient descent

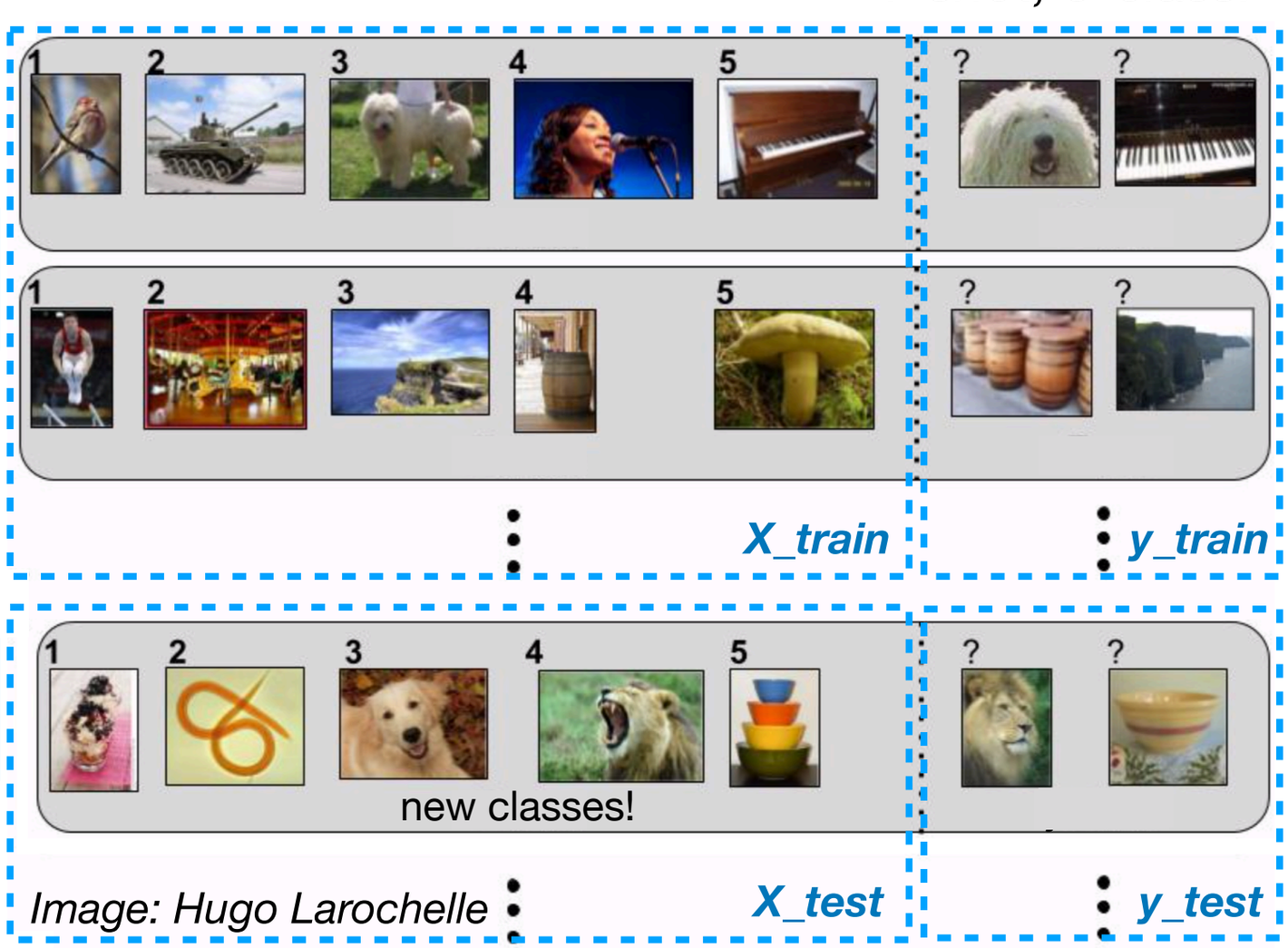
- Left: optimizer and optimizee trained to do style transfer
- Right: optimizer solves similar tasks (different style, content and resolution) without any more training data

Application: Few-shot learning

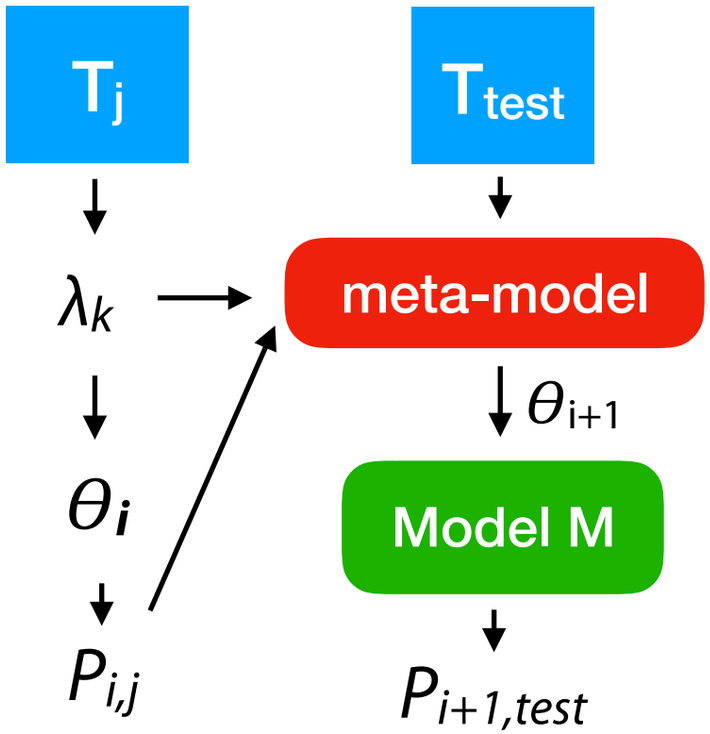
- Learn how to learn from few examples (given similar tasks)
  - Meta-learner must learn how to train a base-learner based on prior experience
    - Parameterize base-learner model and learn the parameters θ_i

$$Cost(\theta_i) = \frac{1}{|T_{test}|} \sum_{t \in T_{test}} loss(\theta_i, t)$$





Few-shot learning: approaches



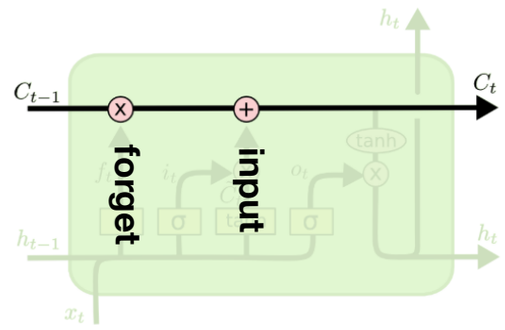
$$Cost(\theta_i) = \frac{1}{|T_{test}|} \sum_{t \in T_{test}} loss(\theta_i, t)$$

- Existing algorithm as meta-learner:
  - LSTM + gradient descent — *Ravi and Larochelle 2017*
  - Learn θ_{init} + gradient descent — *Finn et al. 2017*
  - kNN-like: Memory + similarity — *Vinyals et al. 2016*
  - Learn embedding + classifier — *Snell et al. 2017*
  - …
- Black-box meta-learner
  - Neural Turing machine (with memory) — *Santoro et al. 2016*
  - Neural attentive learner — *Mishra et al. 2018*
  - …

LSTM meta-learner + gradient descent

- Gradient descent update θ_t is similar to LSTM cell state update c_t

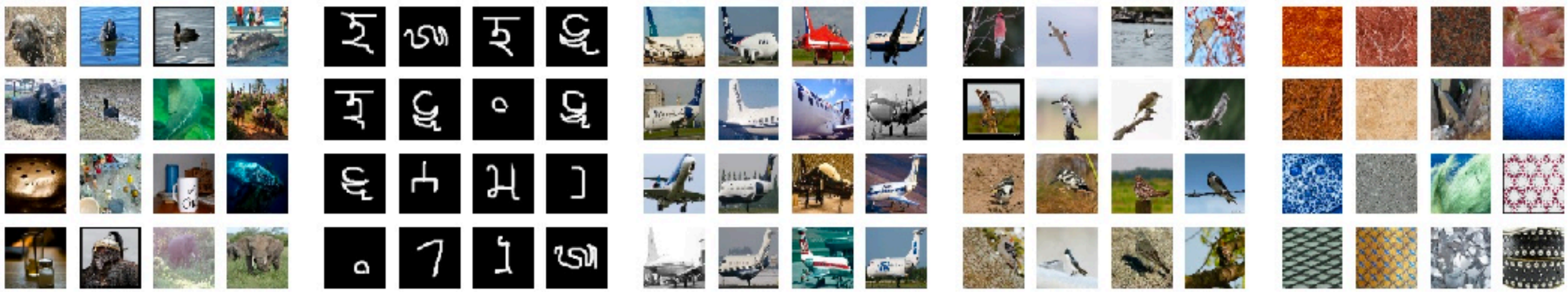
$$\theta_t = \theta_{t-1} - \alpha_t \nabla_{\theta_{t-1}} \mathcal{L}_t \qquad c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t$$



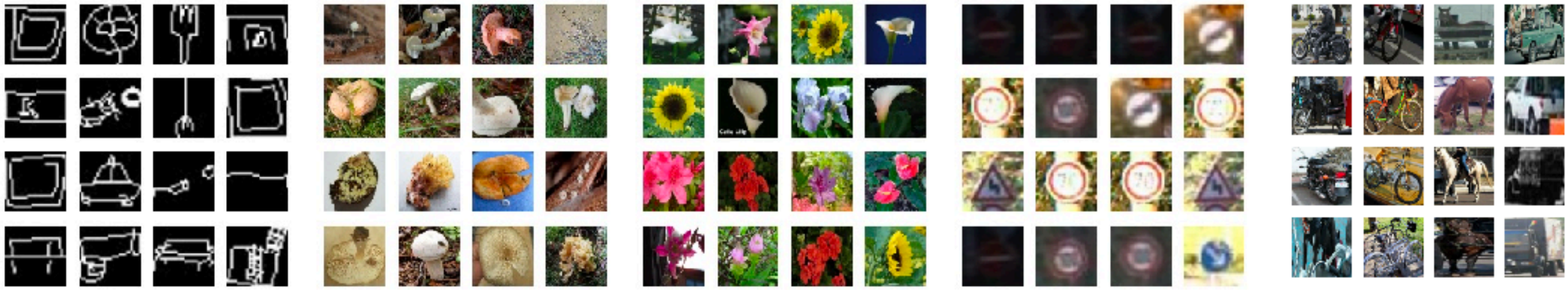
- Hence, training a meta-learner LSTM yields an update rule for training M
  - Start from initial θ_0, train model on first batch, get gradient and loss update
  - Predict θ_{t+1}, continue to t=T, get cost, backpropagate to learn LSTM weights, optimal θ_0

Triantafillou et al. 2019

Meta-dataset



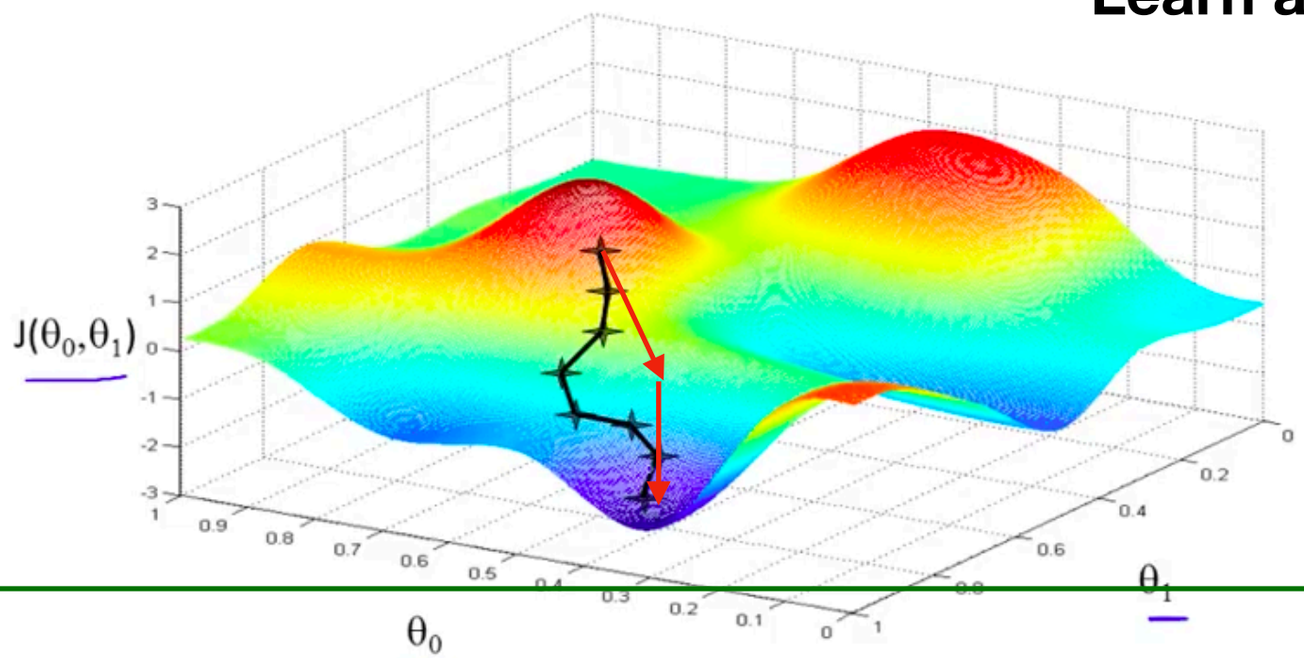
(a) ImageNet (b) Omniglot (c) Aircraft (d) Birds (e) DTD

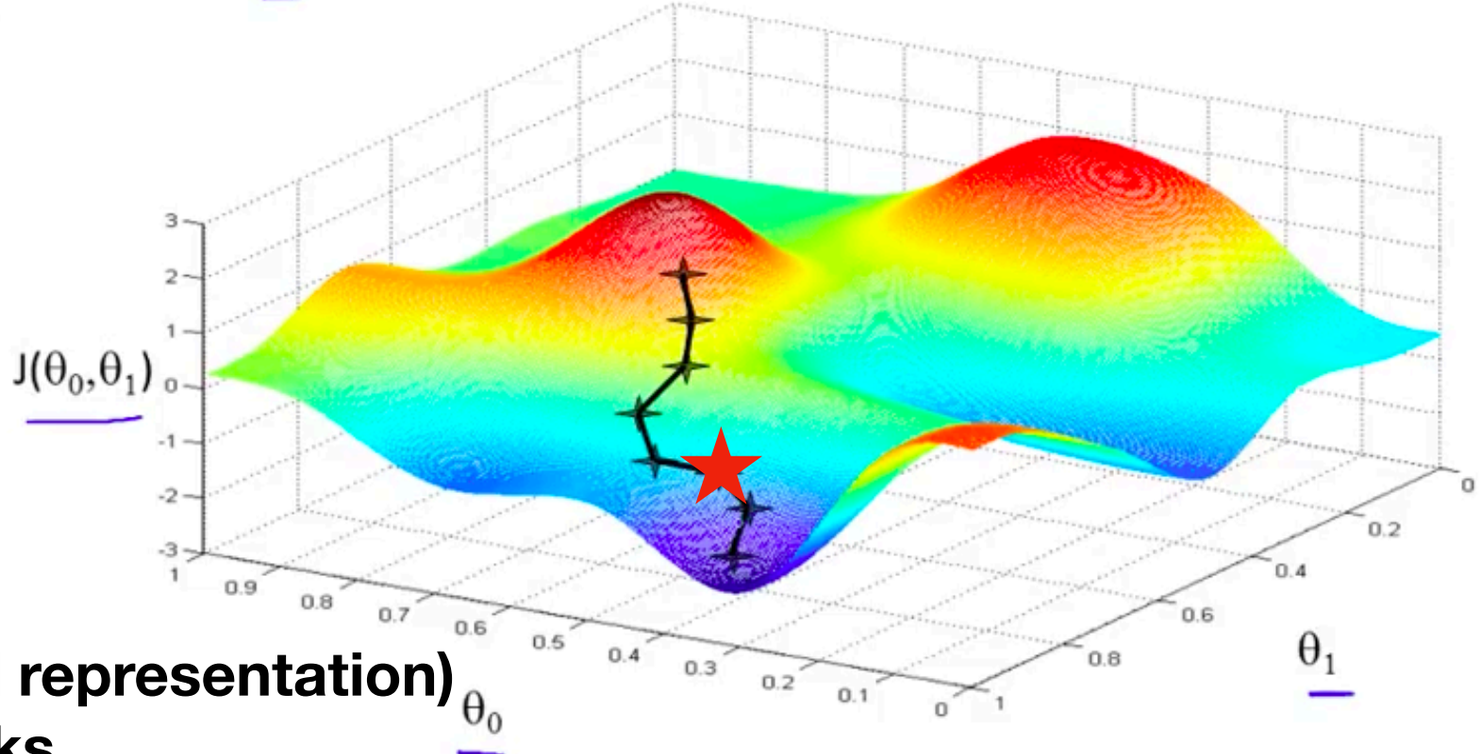


(f) Quick Draw (g) Fungi (h) VGG Flower (i) Traffic Signs (j) MSCOCO

Learning to learn

Learn a better gradient update rule for a group of tasks



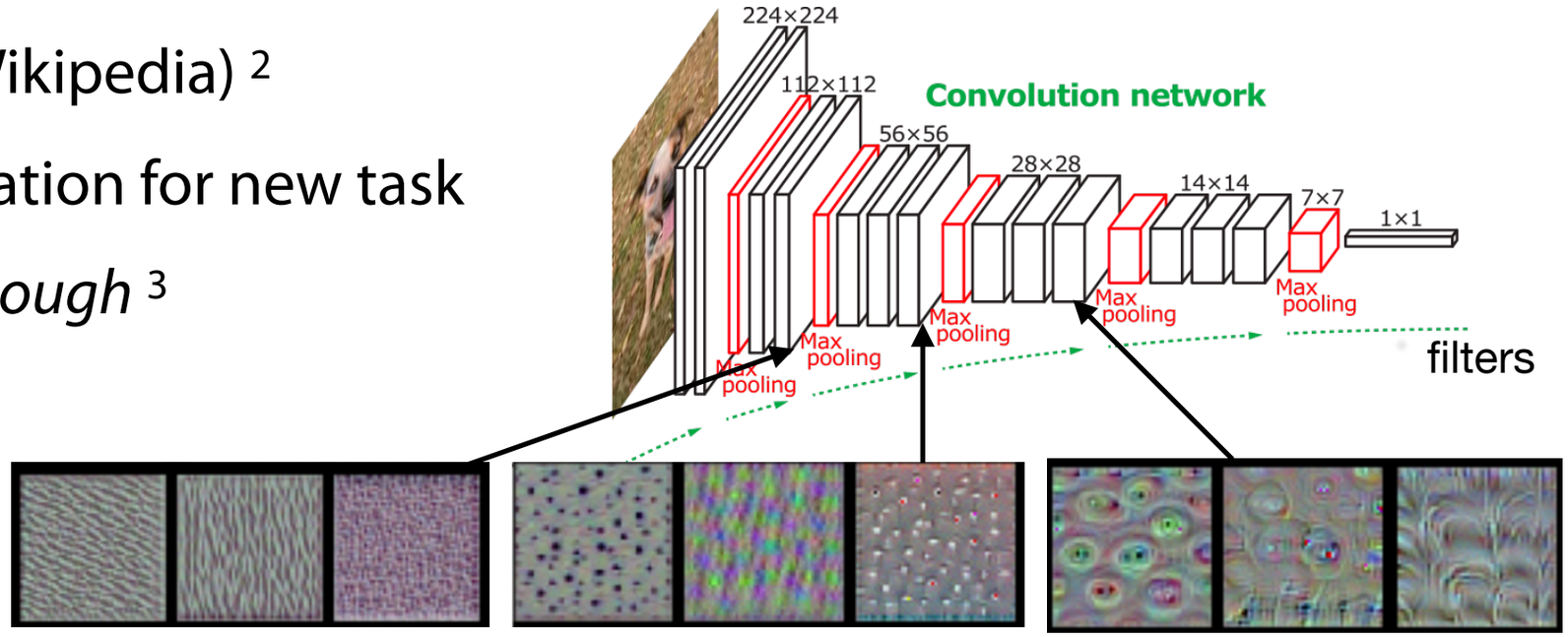


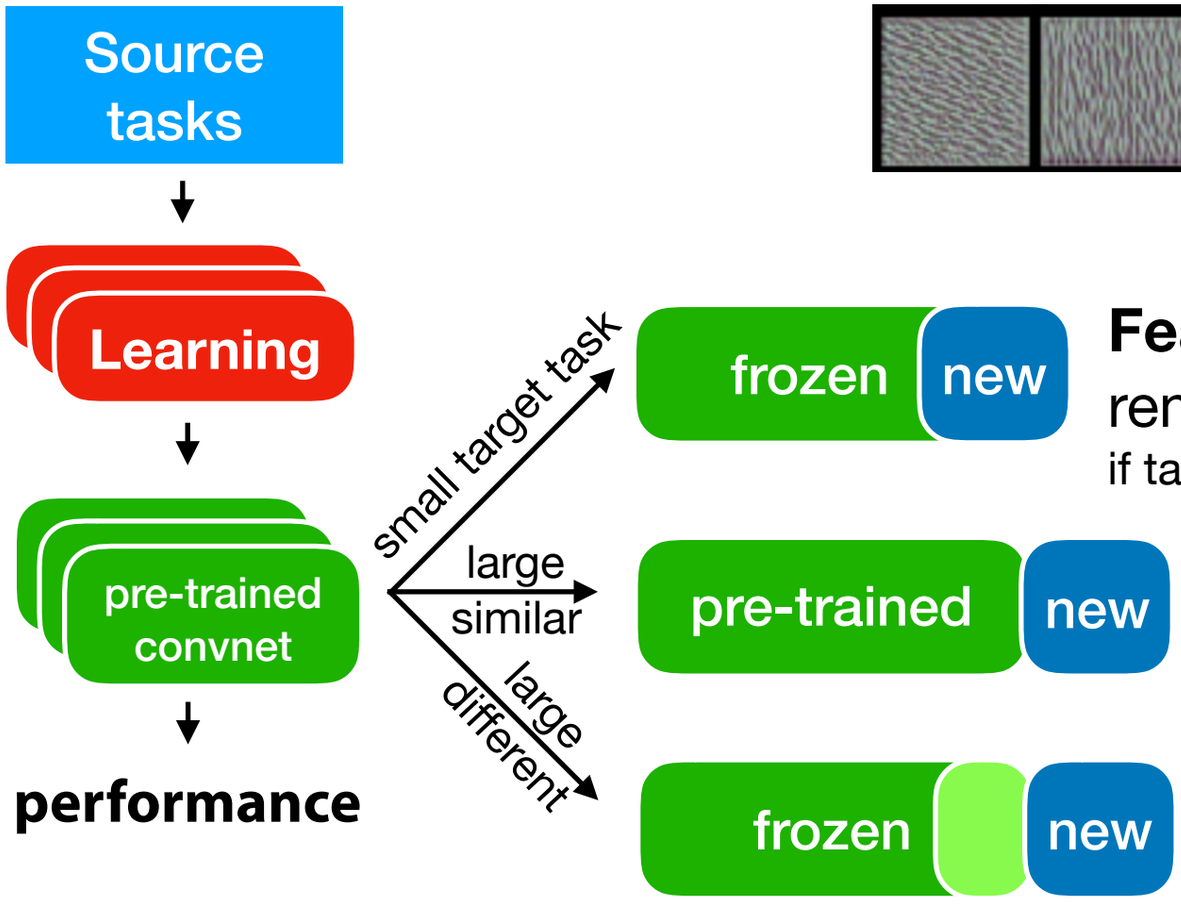
Learn a better initialization (and representation) for a group of tasks

[1] Razavian et al. 2014
[2] Mikolov et al. 2013
[3] Yosinski et al. 2014

Transfer learning

- Pre-train w*eights* from:
  - Large image datasets (e.g. ImageNet) [1]
  - Large text corpora (e.g. Wikipedia) [2]
- Use these weights as initialization for new task
- Fails if tasks are *not similar enough* [3]





Feature extraction:
remove last layers, use output as features
if task is quite different, remove more layers

End-to-end tuning:
train from initialized weights

Fine-tuning:
unfreeze last layers, tune on new task

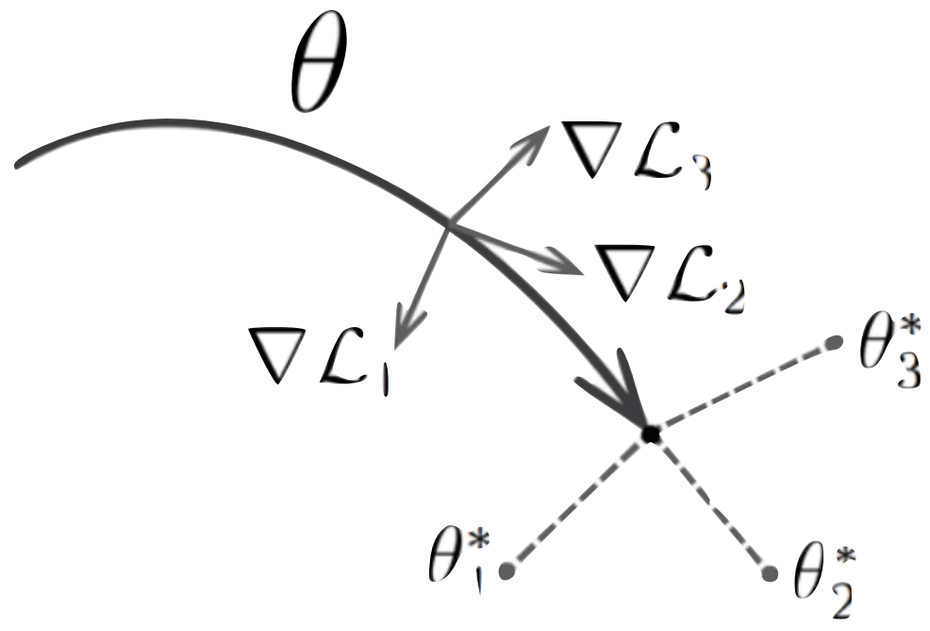
[1] Finn et al. 2017

Model-agnostic meta-learning

- Solve new tasks faster by learning a model *initialization* from similar tasks
  - Current initialization θ
  - On K examples/task, evaluate $\nabla_\theta L_{T_i}(f_\theta)$
  - Update weights for $\theta_1, \theta_2, \theta_3$
  - Update θ to minimize sum of per-task losses

$$\theta \leftarrow \theta - \beta \nabla_\theta \sum_{T_i \sim p(T)} \mathcal{L}_{T_i}\left(f_{\theta_i'}\right)$$

  - Repeat



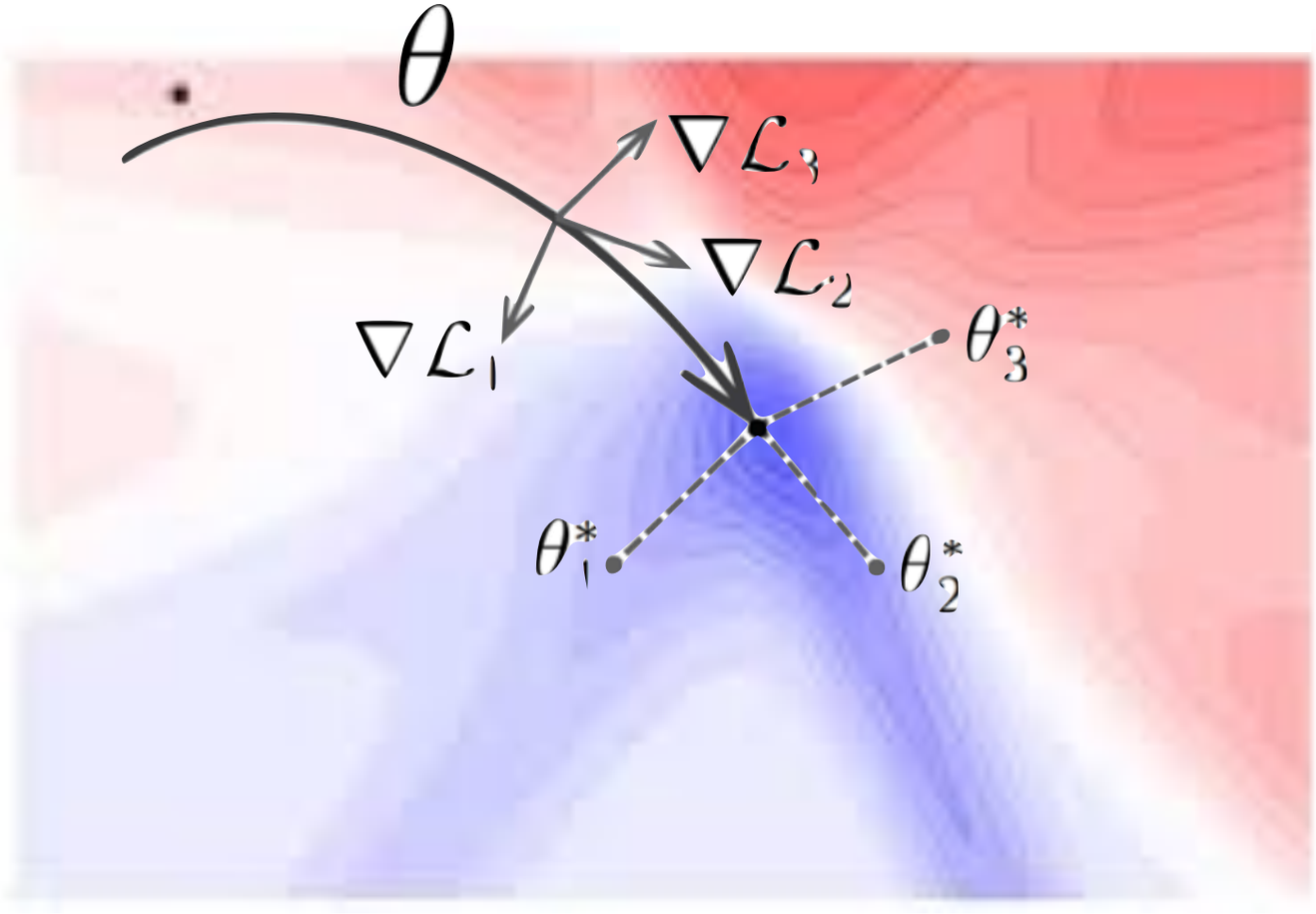
[1] Finn et al. 2017

Model-agnostic meta-learning

- Solve new tasks faster by learning a model *initialization* from similar tasks
  - Current initialization θ
  - On K examples/task, evaluate $\nabla_\theta L_{T_i}(f_\theta)$
  - Update weights for $\theta_1, \theta_2, \theta_3$
  - Update θ to minimize sum of per-task losses

$$\theta \leftarrow \theta - \beta \nabla_\theta \sum_{T_i \sim p(T)} \mathcal{L}_{T_i}\left(f_{\theta_i'}\right)$$

  - Repeat



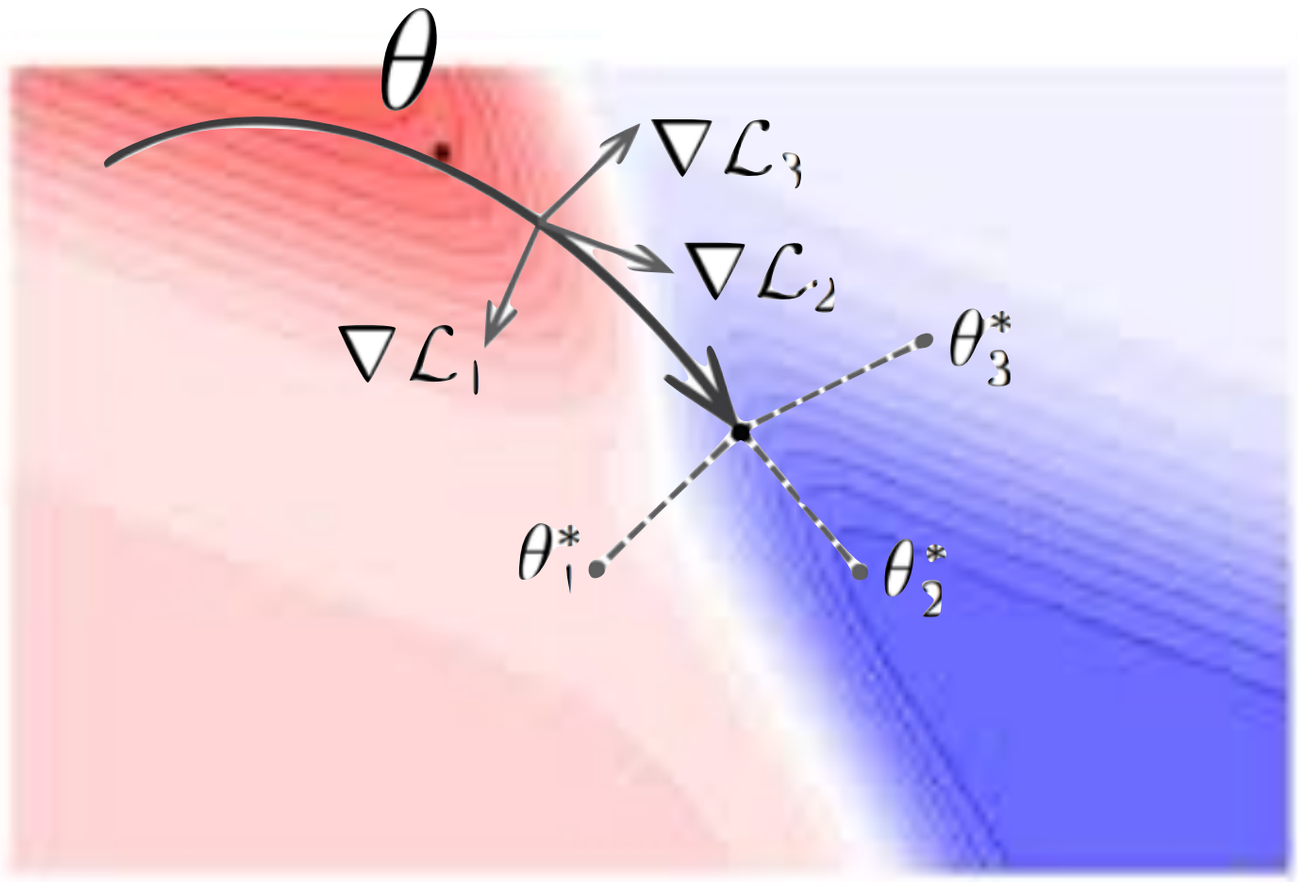
[1] Finn et al. 2017

Model-agnostic meta-learning

- Solve new tasks faster by learning a model *initialization* from similar tasks
  - Current initialization θ
  - On K examples/task, evaluate $\nabla_\theta L_{T_i}(f_\theta)$
  - Update weights for $\theta_1, \theta_2, \theta_3$
  - Update θ to minimize sum of per-task losses

$$\theta \leftarrow \theta - \beta \nabla_\theta \sum_{T_i \sim p(T)} \mathcal{L}_{T_i}\left(f_{\theta_i'}\right)$$

  - Repeat



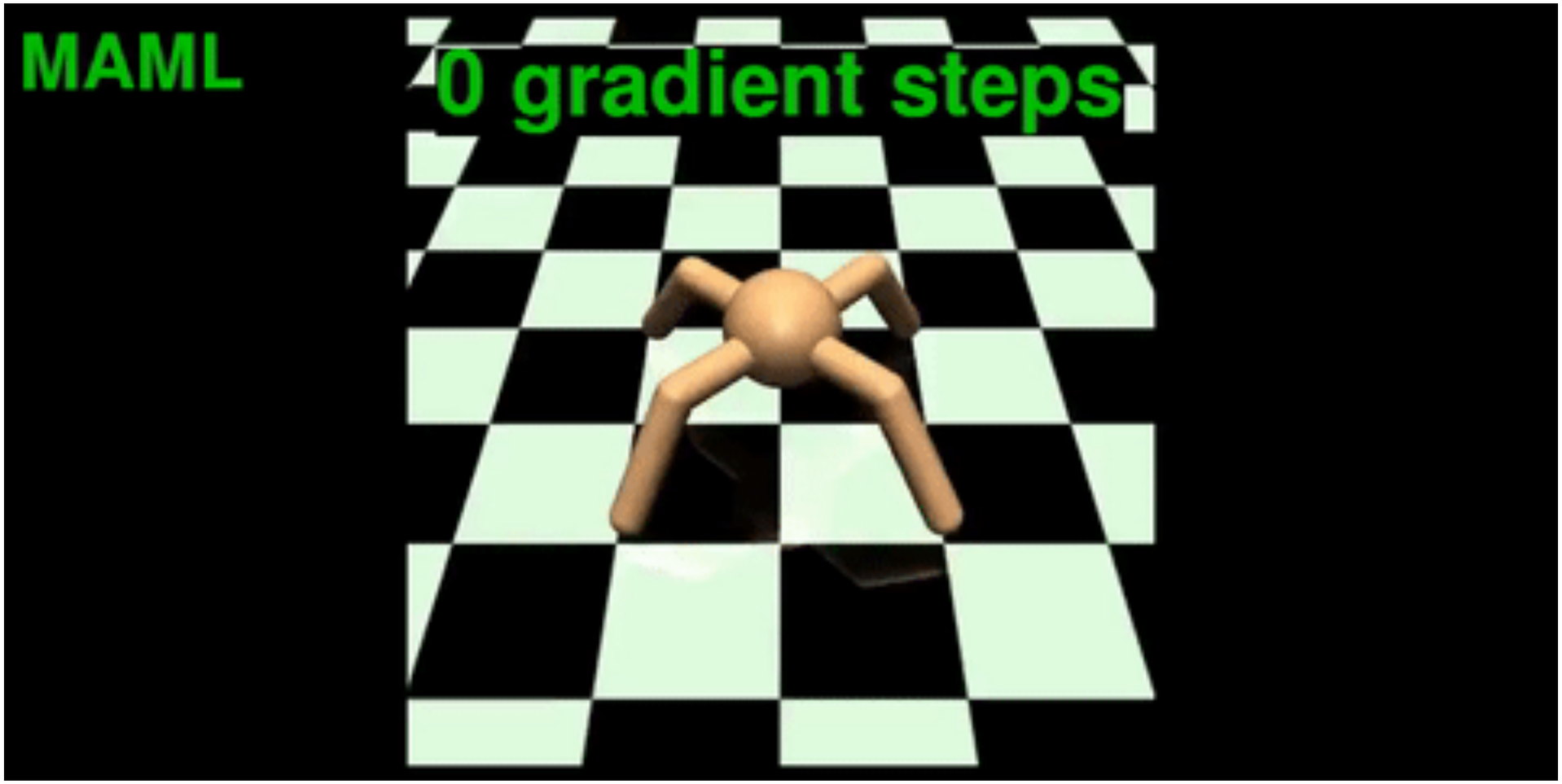
[1] Finn et al. 2018
[2] Nichol et al. 2018

Model-agnostic meta-learning

- More resilient to overfitting
- Generalizes better than LSTM approaches for few shot learning
- *Universality* [1]: no theoretical downsides in terms of expressivity when compared to alternative meta-learning models.
- Many variants and applications: *Finn & Levine 2019*
  - REPTILE: do SGD for k steps in one task, only then update init. weights [2]
  - PLATIPUS: probabilistic MAML
  - Bayesian MAML (Bayesian ensemble)
  - Online MAML
  - …

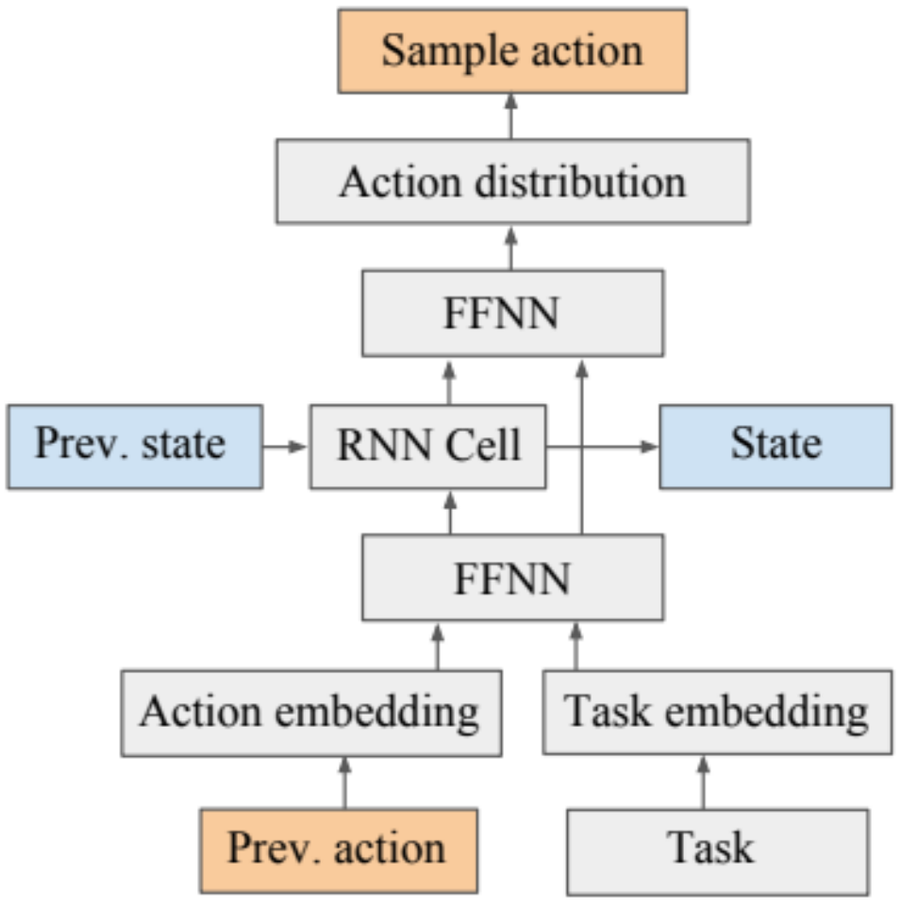
Model-agnostic meta-learning

- For reinforcement learning:



Neural Architecture Meta-Learning

- Warm-start a deep RL controller based on prior tasks *Wong et al. 2018*
- Much faster than single-task equivalent

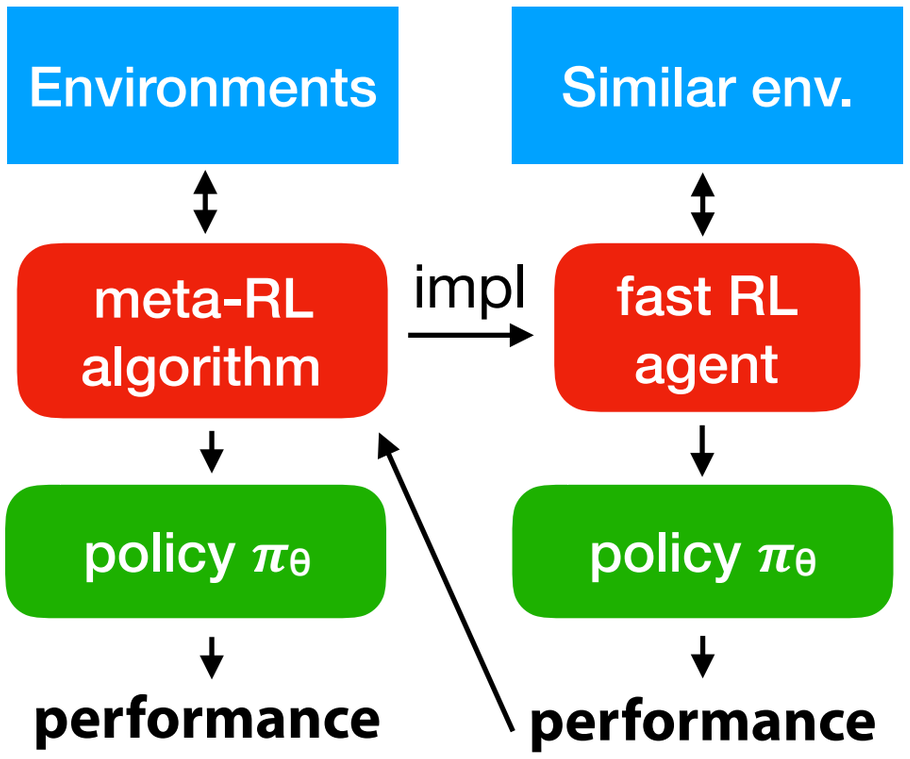


- Another idea: warm-start DARTS with task-specific one-shot model

[1] Duan et al. 2017
[2] Wang et al. 2017
[3] Duan et al. 2017

Learning to reinforcement learn

- Humans often learn to play new games much faster than RL techniques do
- Reinforcement learning is very suited for learning-to-learn:
  - Build a learner, then use performance as that learner as a reward

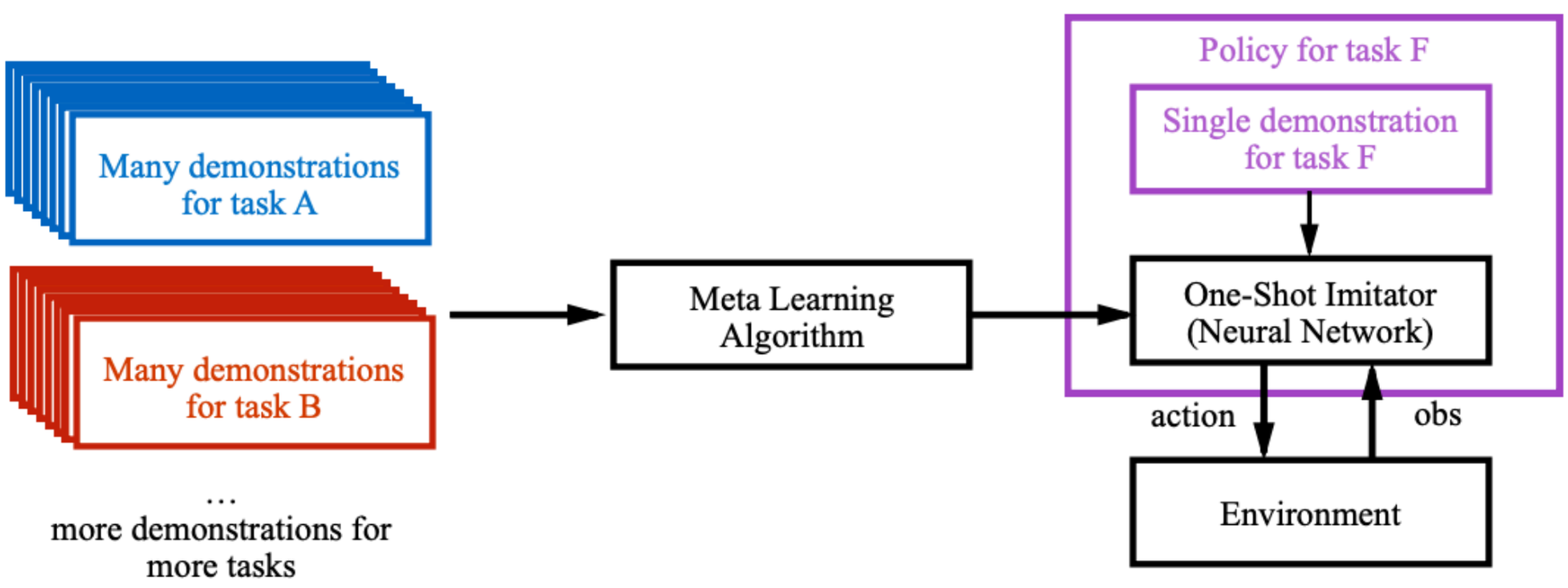


- Learning to reinforcement learn [1,2]
  - Use RNN-based deep RL to train a recurrent network on many tasks
  - Learns to implement a ‘fast’ RL agent, encoded in its weights

[1] Duan et al. 2017
[2] Wang et al. 2017
[3] Duan et al. 2017

Learning to reinforcement learn

- Also works for few-shot learning [3]
  - Condition on observation + upcoming demonstration
- You don't know what someone is trying to teach you, but you prepare for the lesson



Learning to learn more tasks

- Active learning — *Pang et al. 2018*
  - Deep network (learns representation) + policy network
  - Receives state and reward, says which points to query next
- Density estimation — *Reed et al. 2017*
  - Learn distribution over small set of images, can generate new ones
  - Uses a MAML-based few-shot learner
- Matrix factorization — *Vartak et al. 2017*
  - Deep learning architecture that makes recommendations
  - Meta-learner learns how to adjust biases for each user (task)
- Replace hand-crafted algorithms by learned ones.
- Look at problems through a meta-learning lens!

Meta-data sharing building a shared memory

- What if we have a shared memory of all machine learning experiments?
- OpenML.org
  - Thousands of uniform datasets, 100+ meta-features
  - Millions of evaluated runs
    - Same splits, 30+ metrics
    - Traces, models *(opt)*
- **APIs in Python, R, Java,… Sklearn, Keras, PyTorch, MXNet,…**
- Publish your own runs
- **Never ending learning**
- Benchmarks

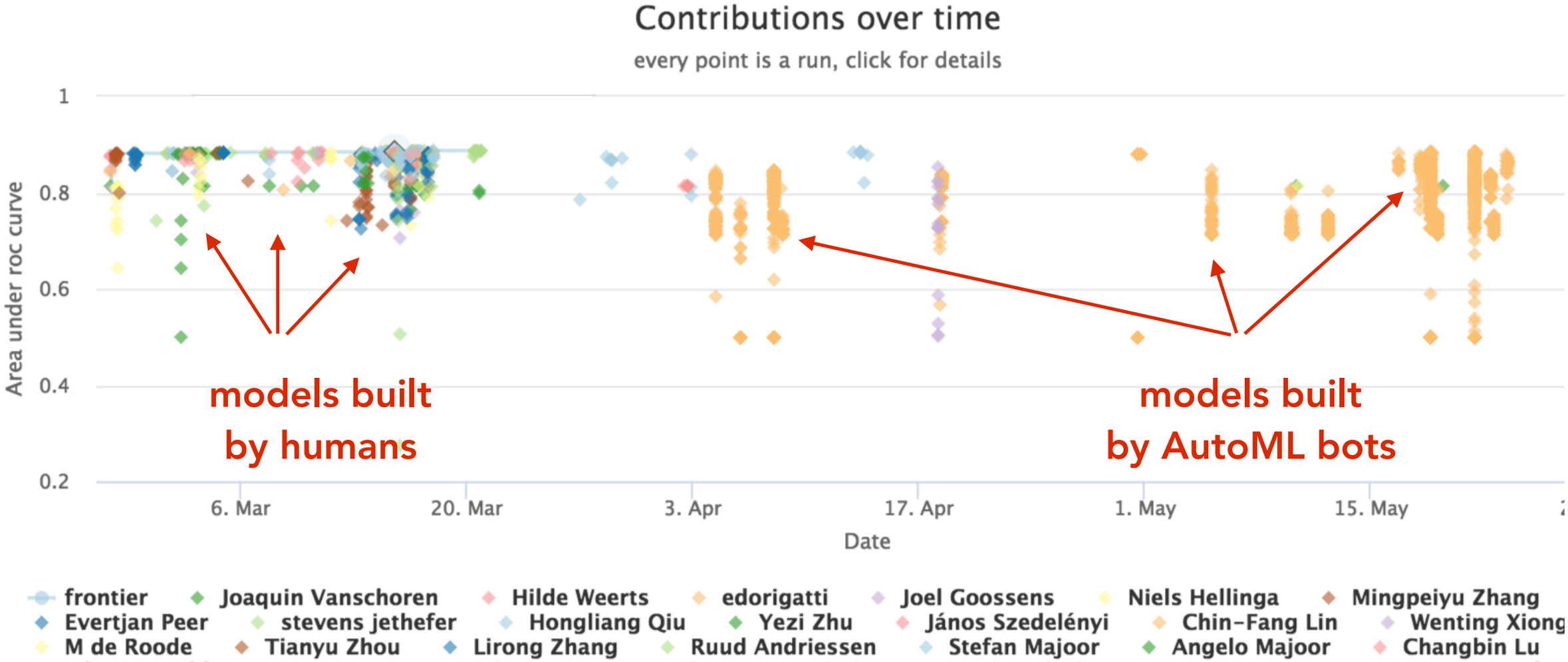
```
import openml as oml
from sklearn import tree

task = oml.tasks.get_task(14951)
clf = tree.ExtraTreeClassifier()
flow = oml.flows.sklearn_to_flow(clf)
run = oml.runs.run_flow_on_task(task, flow)
myrun = run.publish()
```

run *locally*, share *globally*

Meta-data sharing building a shared memory

- Train and run AutoML bots on any OpenML dataset
- Never-ending learning (from robots and humans)

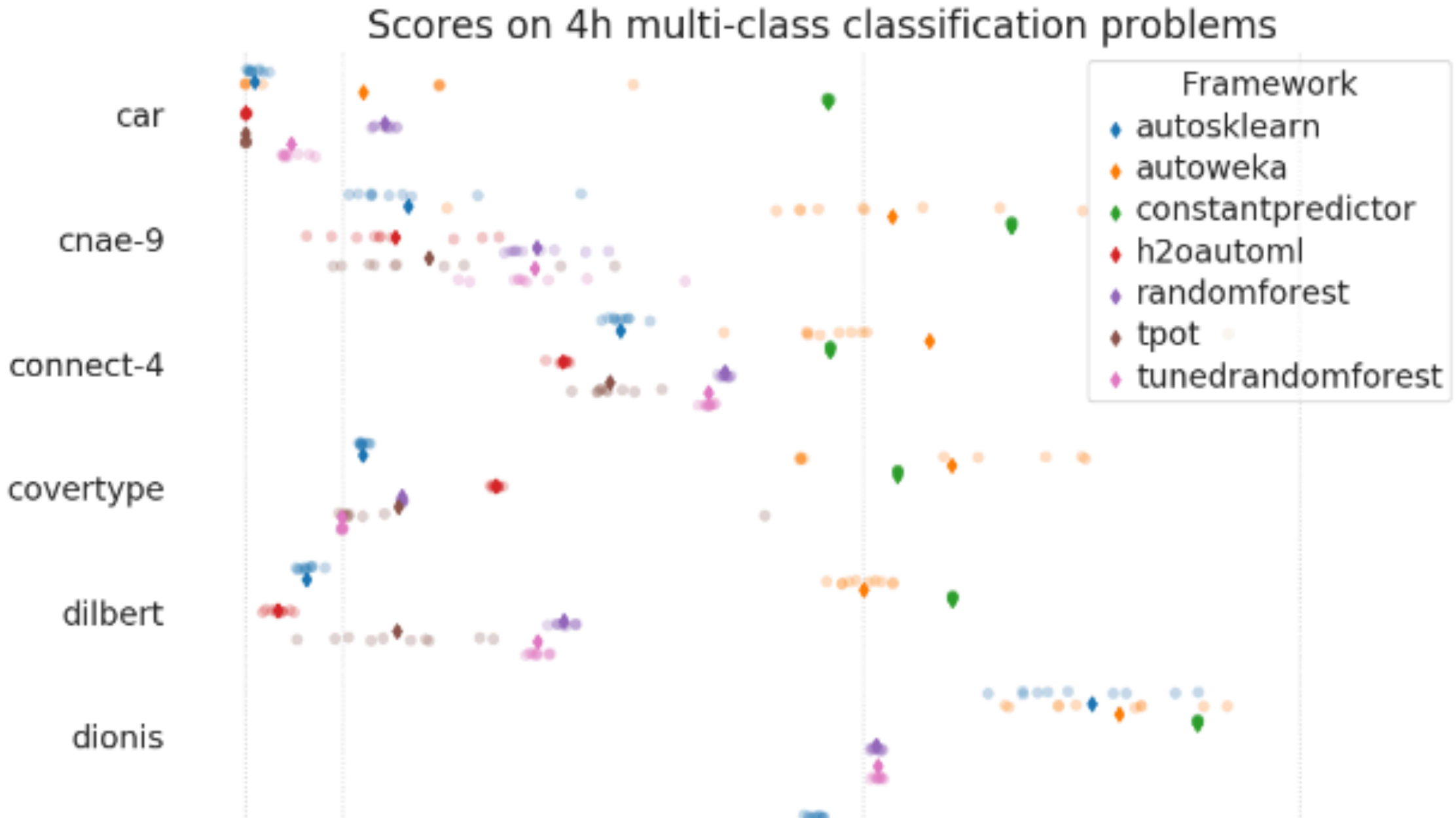


Gijsbers et al. 2019

AutoML tools and benchmarks

Open source benchmark on https://openml.github.io/automlbenchmark/

- On OpenML datasets, will regularly be updated, anyone can add



AutoML open source tools

	Architecture search	Hyperparameter search	Improvements	Meta-learning
Auto-WEKA	Parameterized pipeline	Bayesian Optimization (RF)		
auto-sklearn	Parameterized pipeline	Bayesian Optimization (RF)	Ensembling	warm-start
BO-HB	Parameterized pipeline	Tree of Parzen Estimators	Ensembling, Hyperband	
hyperopt-sklearn	Parameterized pipeline	Tree of Parzen Estimators		
TPOT	Evolving pipelines (trees)	Genetic programming		
GAMA	Evolving pipelines (trees)	Asynchronous evolution	Ensembling, Hyperband	
H2O AutoML	Single algorithms	random search	Stacking	
ML-Plan	Planning-based pipeline	Hierarchical planner		
OBOE	Single algorithms	Low rank approximation	Ensembling	Runtime predictor

AutoML tools and benchmarks

Observations so far (for pipeline search):

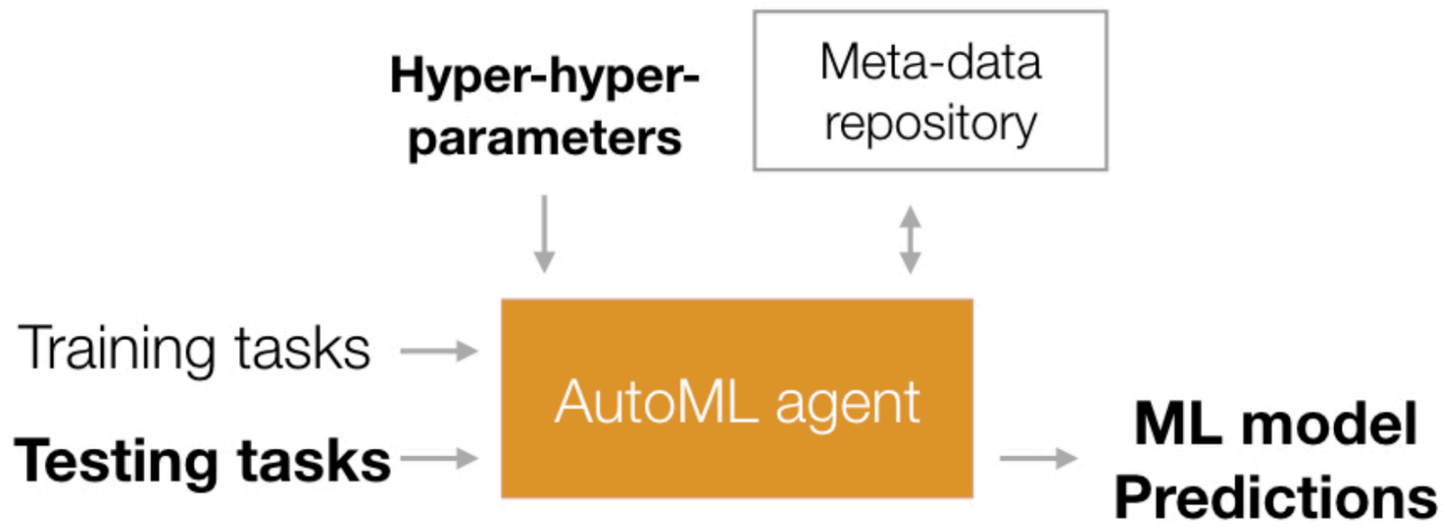
- No AutoML system outperforms all others (Auto-WEKA is worse)
- Auto-sklearn, H2O, TPOT can outperform each other on given datasets
- Tuned RandomForests are a strong baseline
- High numbers of classes, unbalanced classes, are a problem for most tools
- Little support for anytime prediction …

We need good benchmarks for NAS as well…

AutoML Gym

Environment to train general-purpose AutoML algorithms

- Open benchmark, meta-learning, continual learning, efficient NAS



Open PostDoc position!
http://bit.ly/automl-gym

Towards human-like learning to learn

- Learning-to-learn gives humans a significant advantage
  - **Learning how to learn any task empowers us far beyond knowing how to learn specific tasks.**
  - It is a **universal** aspect of life, and how it evolves
- Very exciting field with many unexplored possibilities
  - Many aspects not understood (e.g. task similarity), need more experiments.
- **Challenge**:
  - Build learners that **never stop learning**, that **learn from each other**
  - *Fast* learning by *slow* meta-learning
  - Build a ***global memory*** for learning systems to learn from
  - **Let them explore / experiment by themselves**

Thank you!

Never stop learning

more to learn

http://www.automl.org/book/

Chapter 2: Meta-Learning

special thanks to

Pavel Brazdil, Matthias Feurer, Frank Hutter, Erin Grant, Hugo Larochelle, Raghu Rajan, Jan van Rijn, Jane Wang