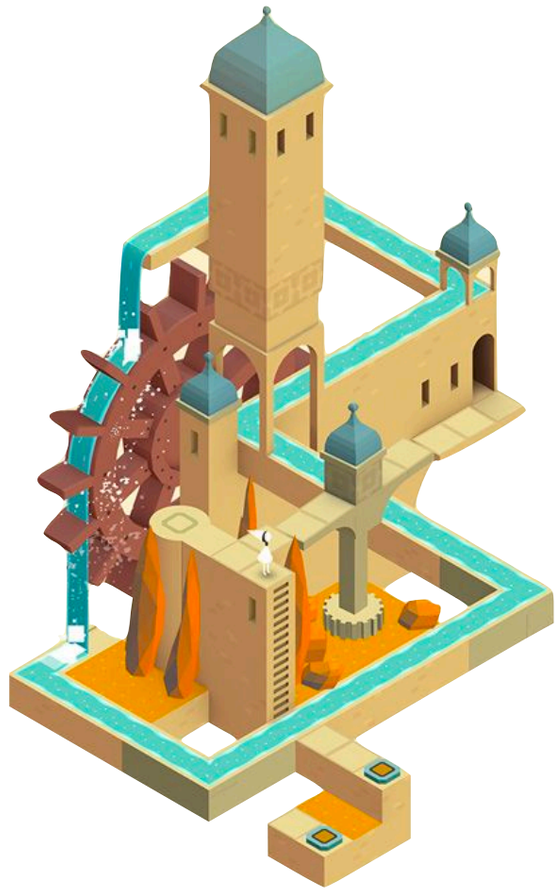

Automatic Machine Learning

A Tutorial

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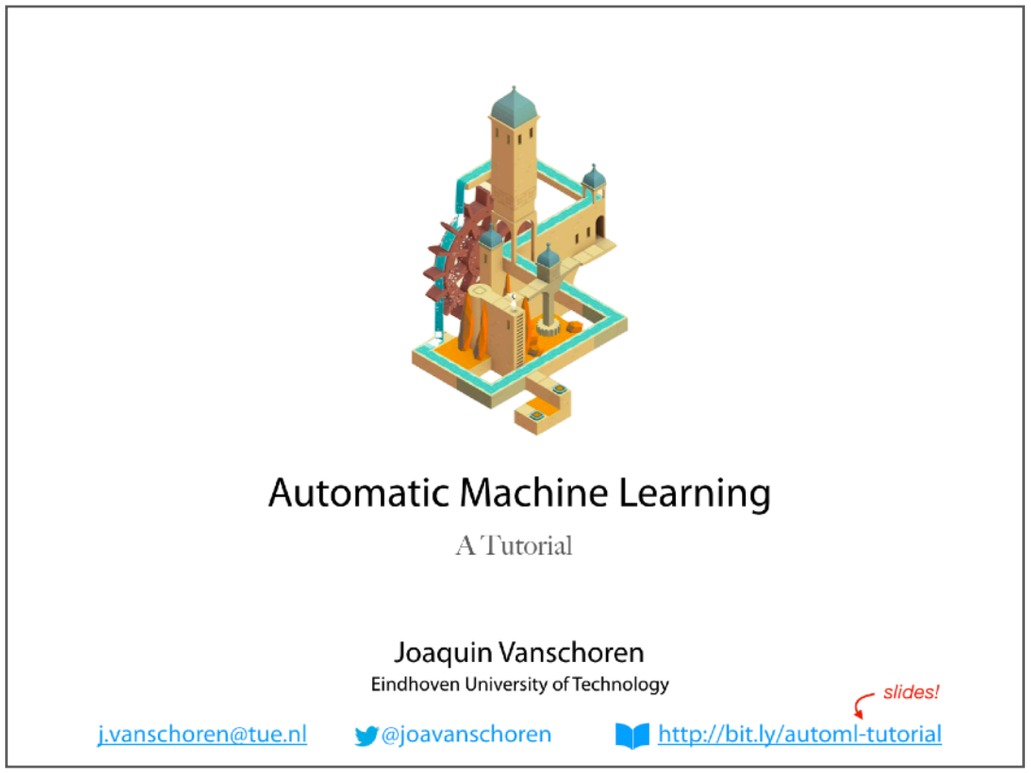
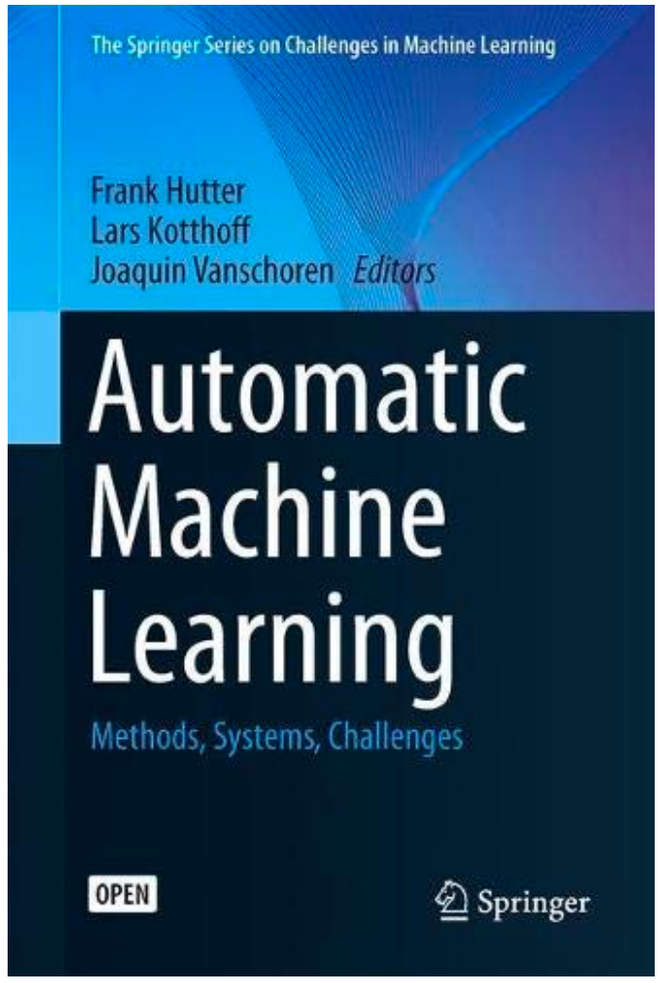
slides!

http://bit.ly/automl-tutorial

Slides / Book



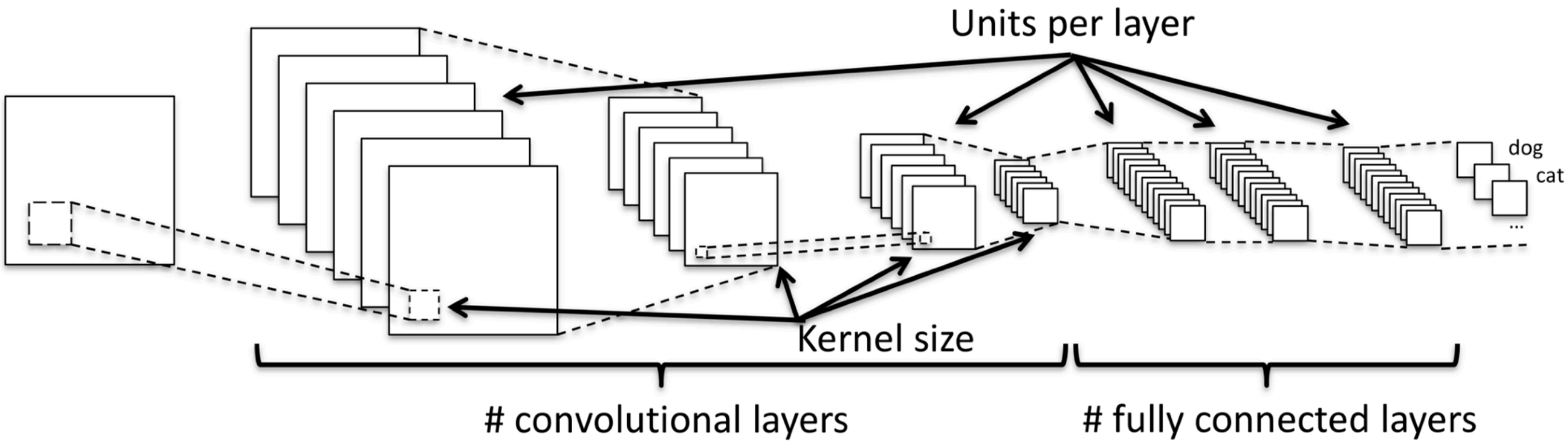
Slides
http://bit.ly/automl-tutorial



Open access book
(free PDF)
www.automl.org/book
www.amazon.de/dp/3030053172

Deep learning requires a lot of expertise

Designing neural architectures

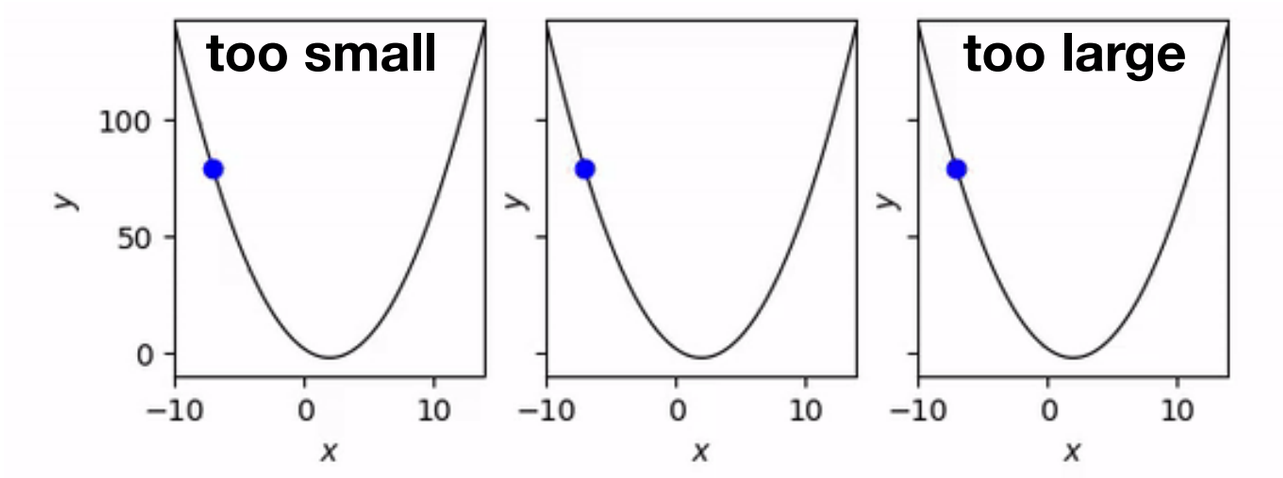


- Choose operators (layers), data preparation, data augmentation, hyperparameter tuning, regularization, early stopping,…

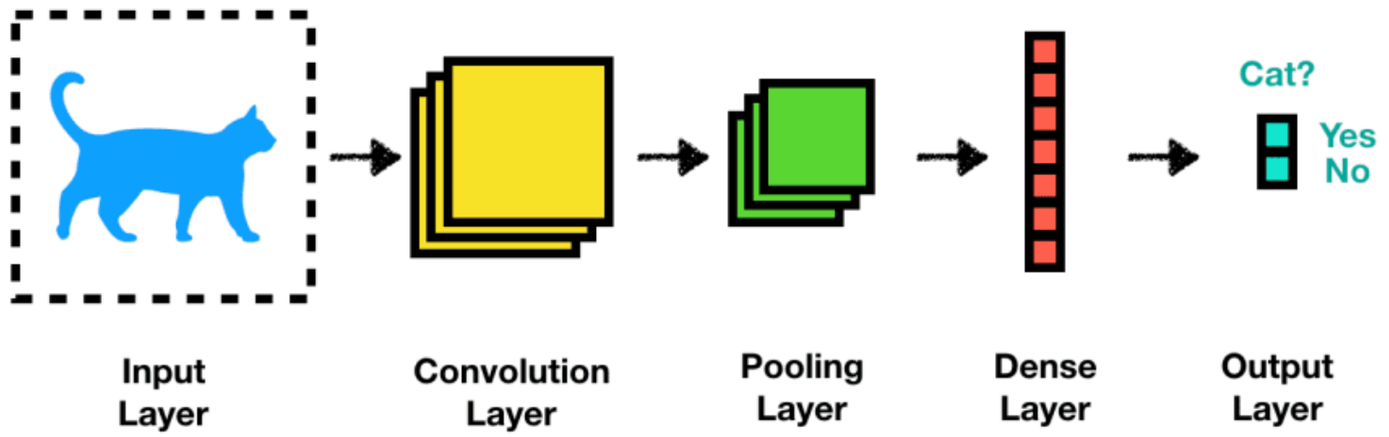
Hyperparameters

Every design decision made by the *user (architecture, operators, tuning,…)*

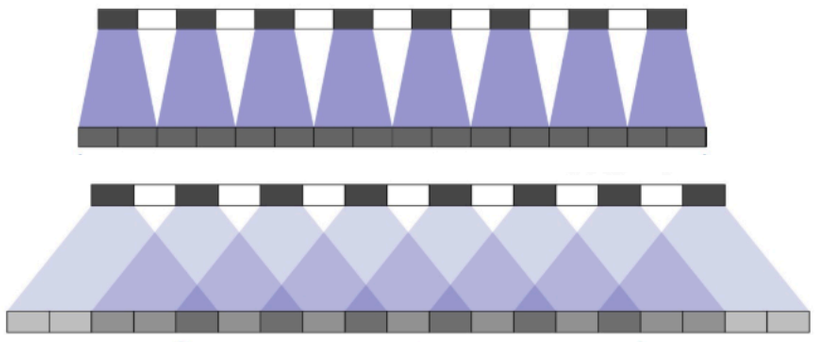
- Numeric
  - e.g. learning rate



- Categorical
  - e.g. layer type



- Conditional
  - ConvLayer -> filter size, stride length,…



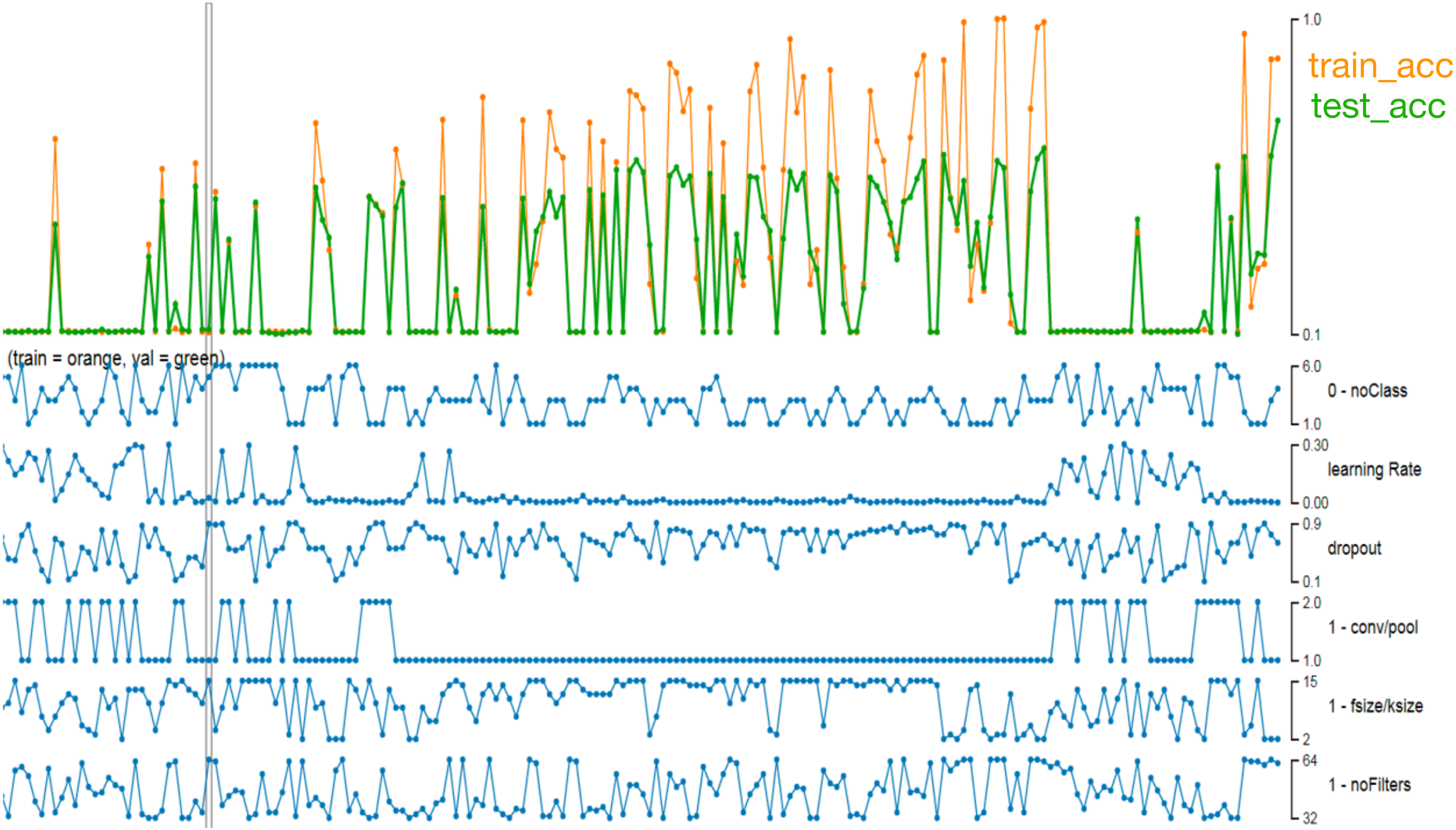
Filter size 2, stride length 2

Filter size 5, stride length 2

Hyperparameters

Some are very sensitive, others not, lots of interactions

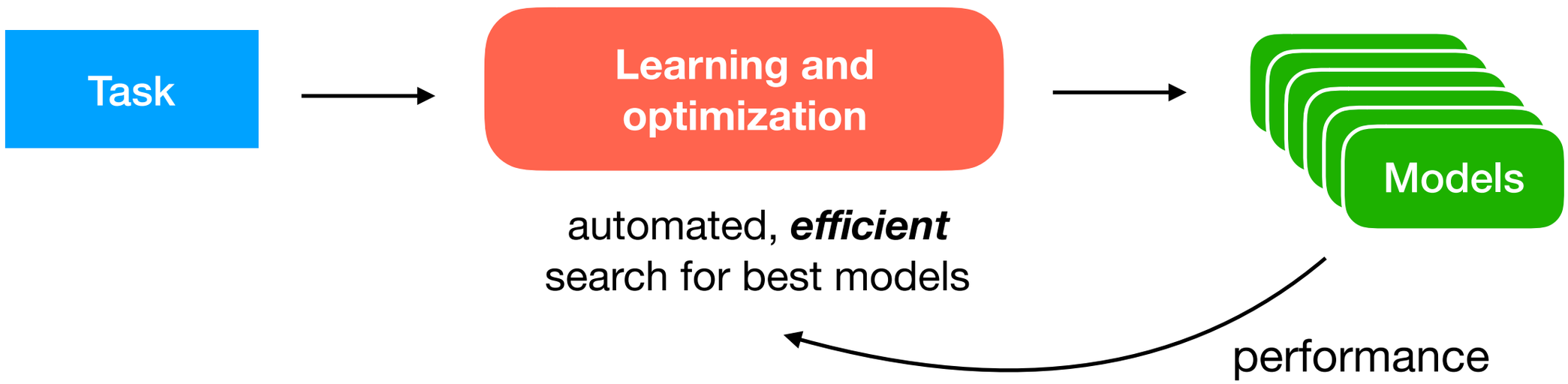
What is the right strategy to find the right configuration?



Automated machine learning

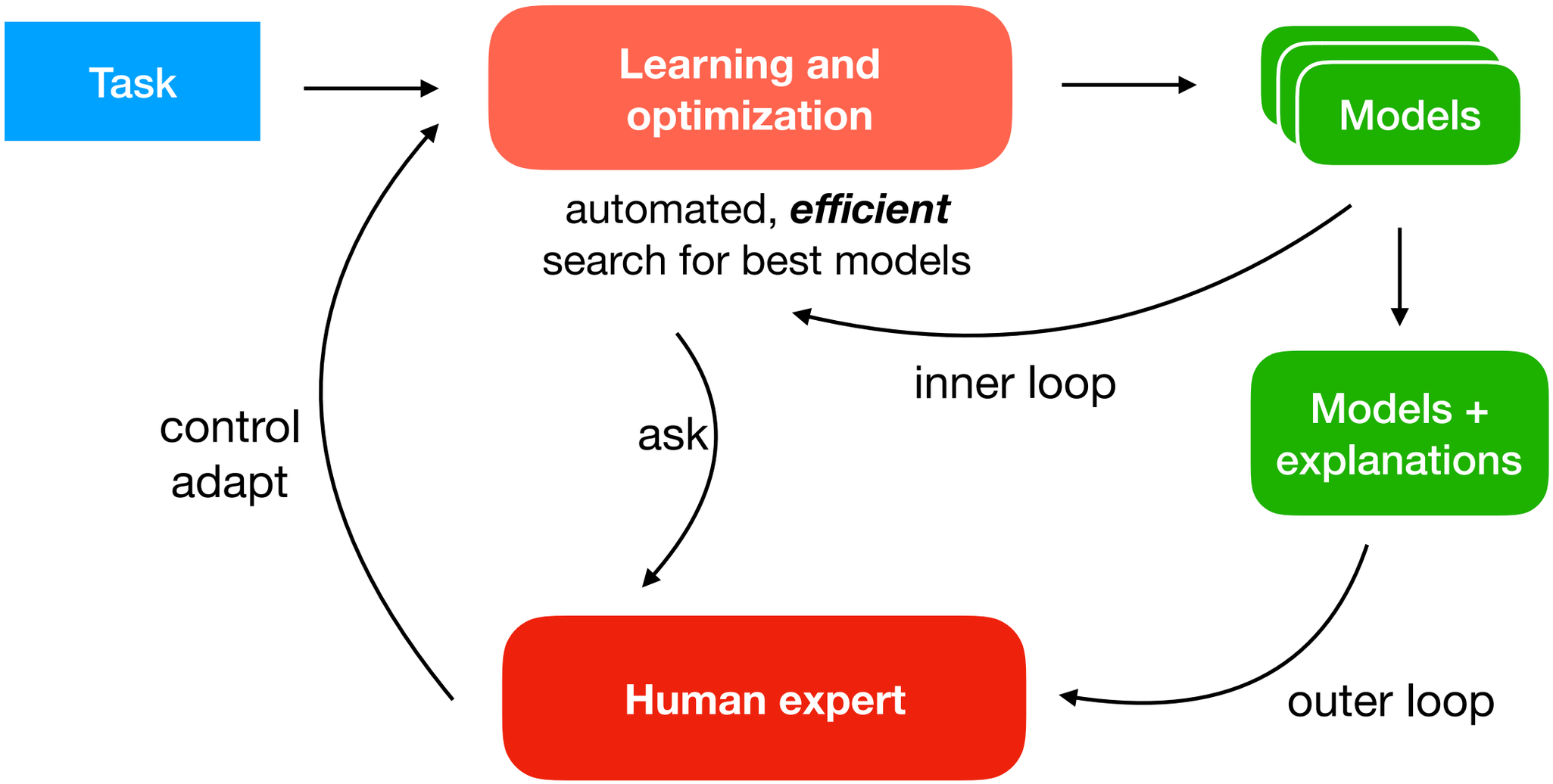
Manual machine learning

AutoML: build models in a data-driven, objective, and automated way



Semi-Automated machine learning

Human-in-the-loop



Domain knowledge and human expertise are very valuable
e.g. unknown unknowns, preference learning,…

Automated machine learning

Today when scientists talk of artificial intelligence, they generally mean 'the art of creating machines that perform functions which require intelligence when performed by people.'"

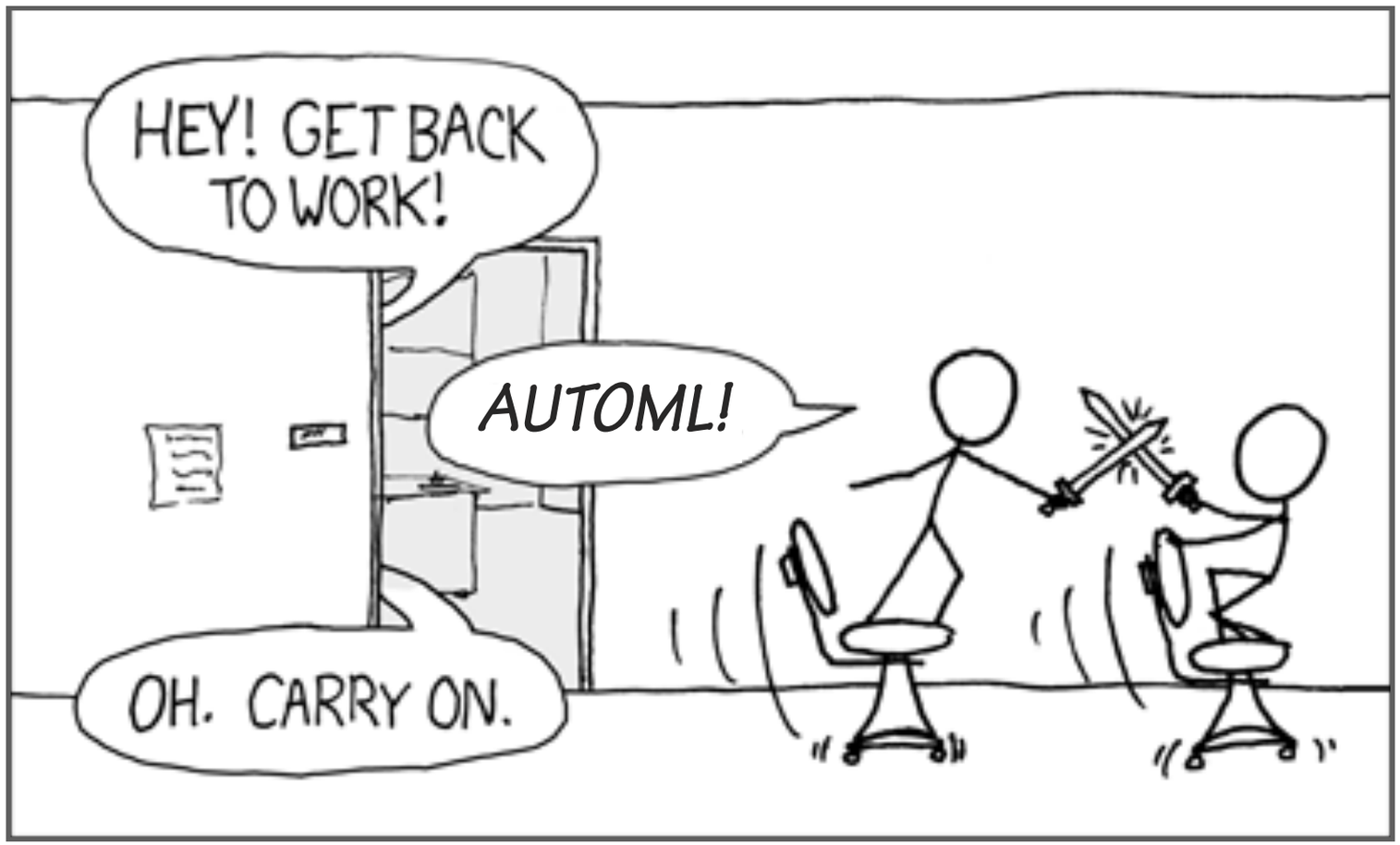
– J. Rifkin

Automated AI is the art of creating machines that perform functions which require intelligence when people build artificial intelligence

… but not all functions.

– J. Vanschoren ;)

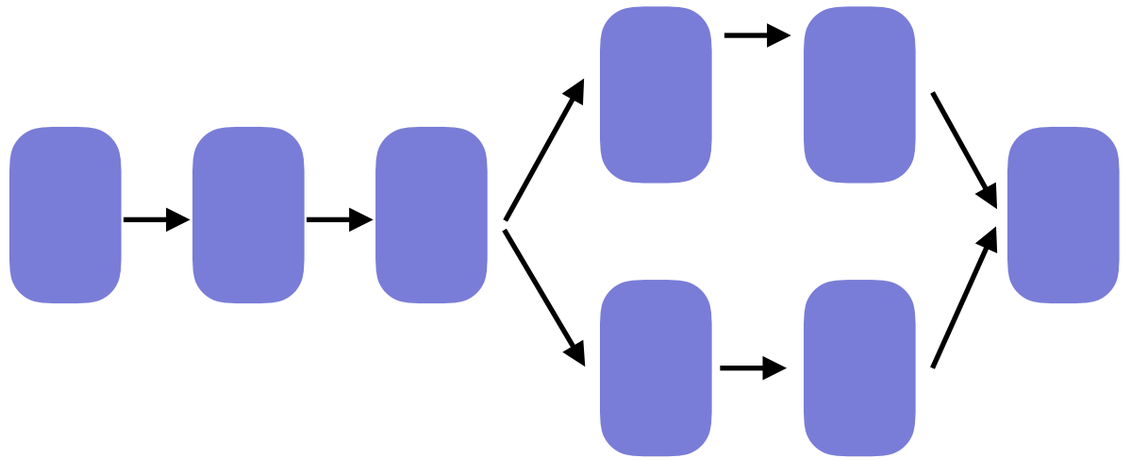
THE DATA SCIENTIST'S #1 EXCUSE FOR LEGITIMATELY SLACKING OFF: "THE AUTOML TOOL IS OPTIMIZING MY MODELS!"



Adapted from XKCD (Randall Munroe)

AutoML: subproblems

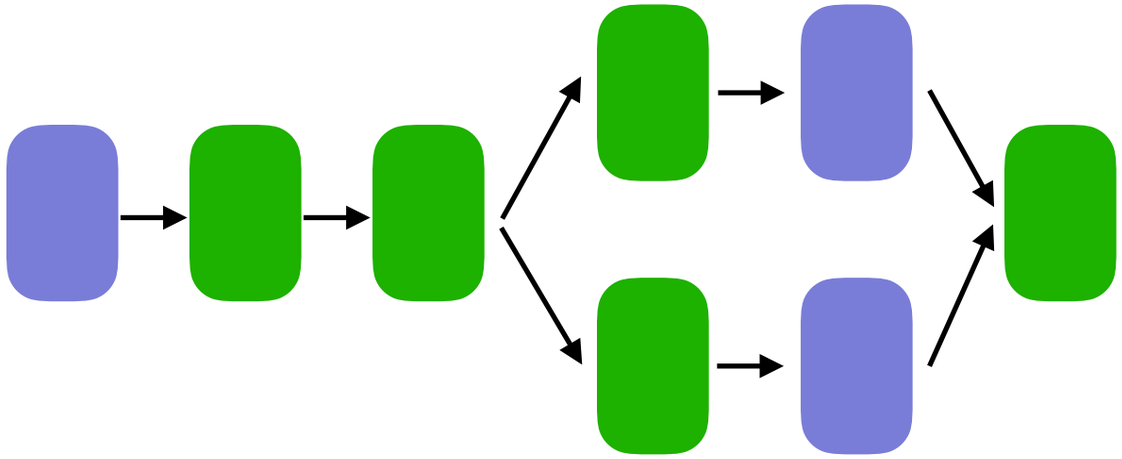
- **Architecture search**: *represent* and search possible architectures
  - Neural layers, branching, skip connections,…
  - Defines the search space



```
model.add(Conv2D(32, (3, 3))
model.add(MaxPooling2D((2, 2)))
model.add(Conv2D(64, (3, 3))
model.add(MaxPooling2D((2, 2)))
model.add(Conv2D(64, (3, 3))
```

AutoML: subproblems

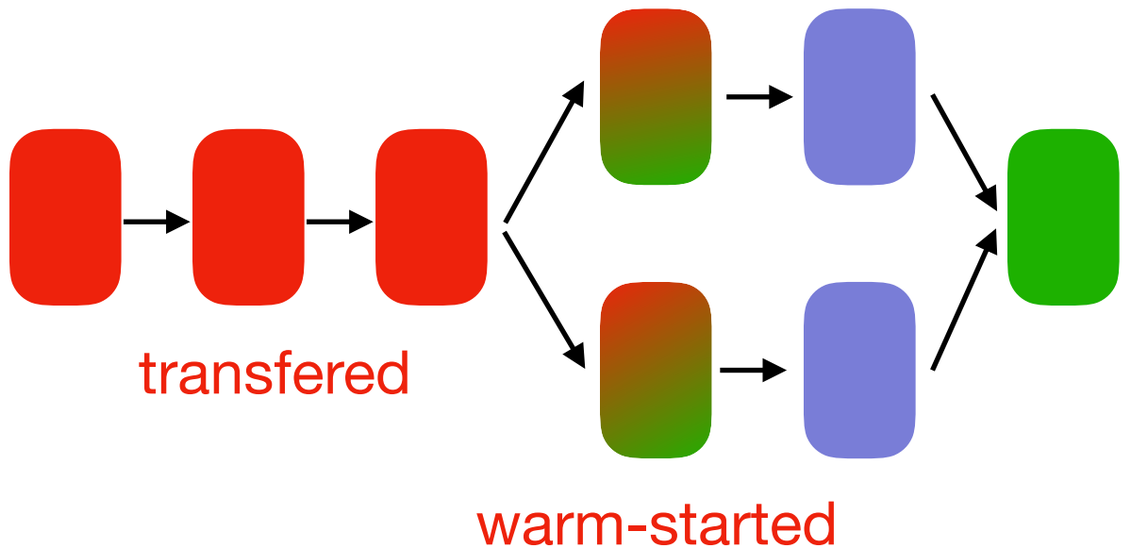
- **Architecture search**: *represent* and search all possible architectures
- **Hyperparameter optimization**:
  - Which hyperparameters are important? How to optimize them?
  - What is the (multi-)objective function?



```
def build_model(hp){
    model.add(Dense(units=hp.Int('units', min_value=32, max_value=512, step=32)))
    model.compile(optimizer=Adam(hp.Choice('learning rate', [1e-2, 1e-3, 1e-4])))
    return model;}
tuner = RandomSearch(build_model, max_trials=5)   //or HyperBand
```

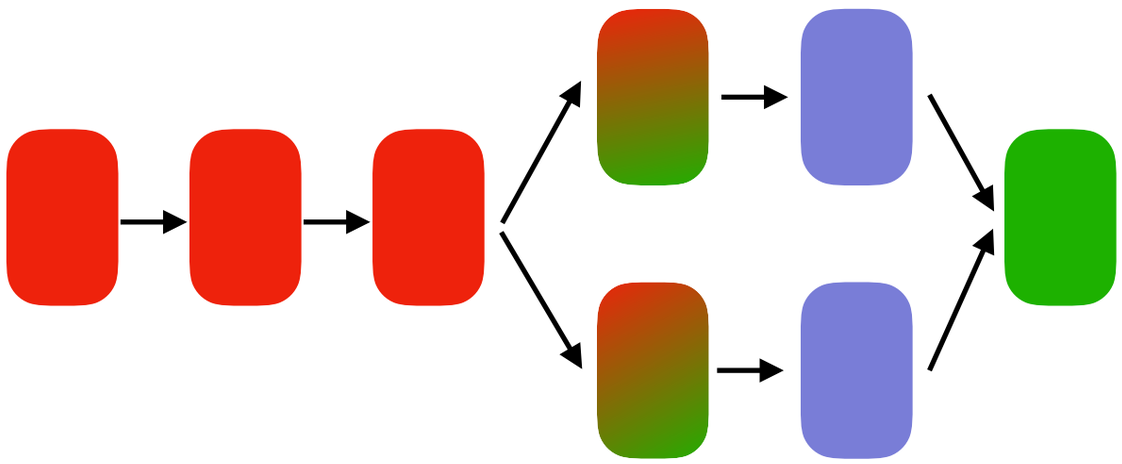
AutoML: subproblems

- **Architecture search**: *represent* and search all possible architectures
- **Hyperparameter optimization**: *optimize* important hyperparameters
- **Meta-learning**: how can we transfer experience from previous tasks?
  - Transfer learning: reuse good architectures/configurations
  - Warm starting: start search from promising architectures/configurations
  - …



AutoML: subproblems

- **Architecture search**: *represent* and search all possible architectures
- **Hyperparameter optimization**: *optimize* remaining hyperparameters
- **Meta-learning**: how can we transfer experience from previous tasks?
  - Don't start from scratch every time



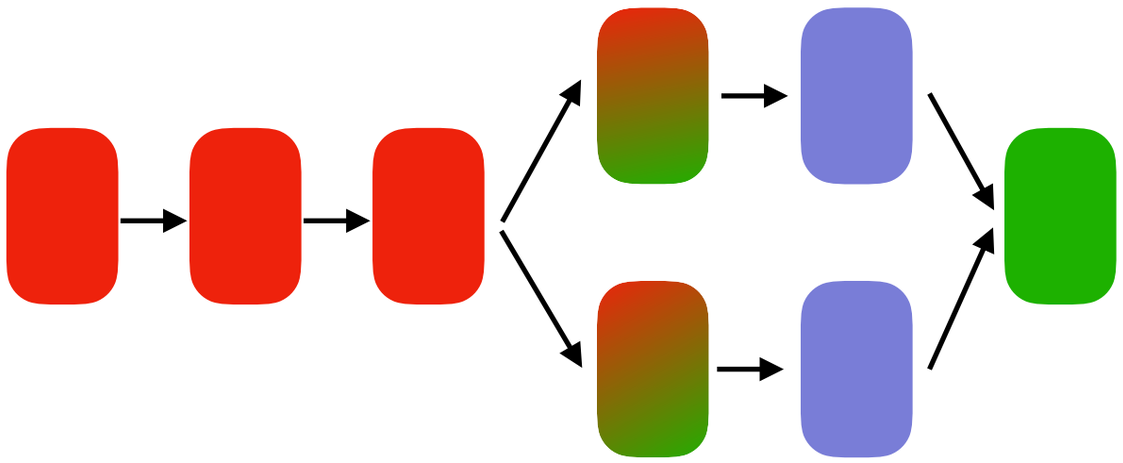
Goal:

```
model = AutoML_Learner().fit(X_train,y_train)
model2 = AutoML_Learner().fit(X2_train,y2_train)
```

meta-learn

AutoML: subproblems

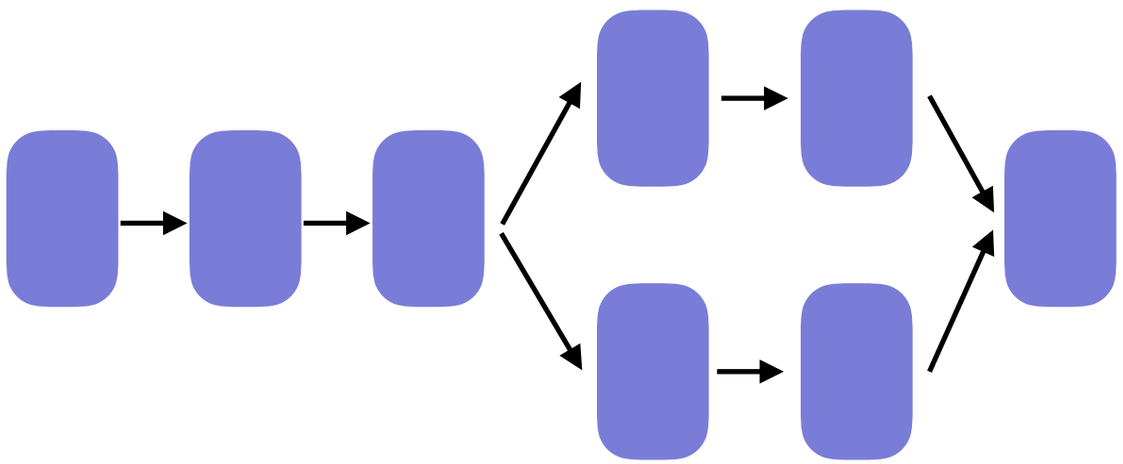
- **Architecture search**: *represent* and search all possible architectures
- **Hyperparameter optimization**: *optimize* remaining hyperparameters
- **Meta-learning**: how can we transfer experience from previous tasks?
  - Don't start from scratch every time



these 3 subproblems can be solved
consecutively, *simultaneously* or *interleaved*

AutoML: subproblems

- **Architecture search**: *many different approaches*
  - Parameterized (fixed) architectures
  - Reinforcement learning
  - Evolution
  - Network morphisms
  - …



Elsken et al. 2019

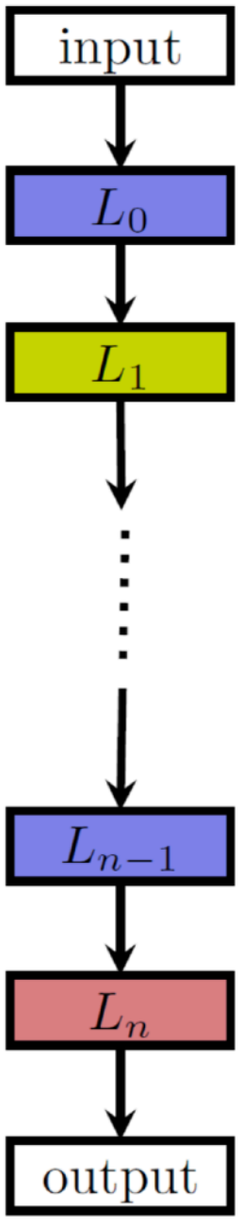
Parameterized architectures

- Fixed (linear) architecture, all possible choices encoded as extra hyperparameters

Parameterized Sequential

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

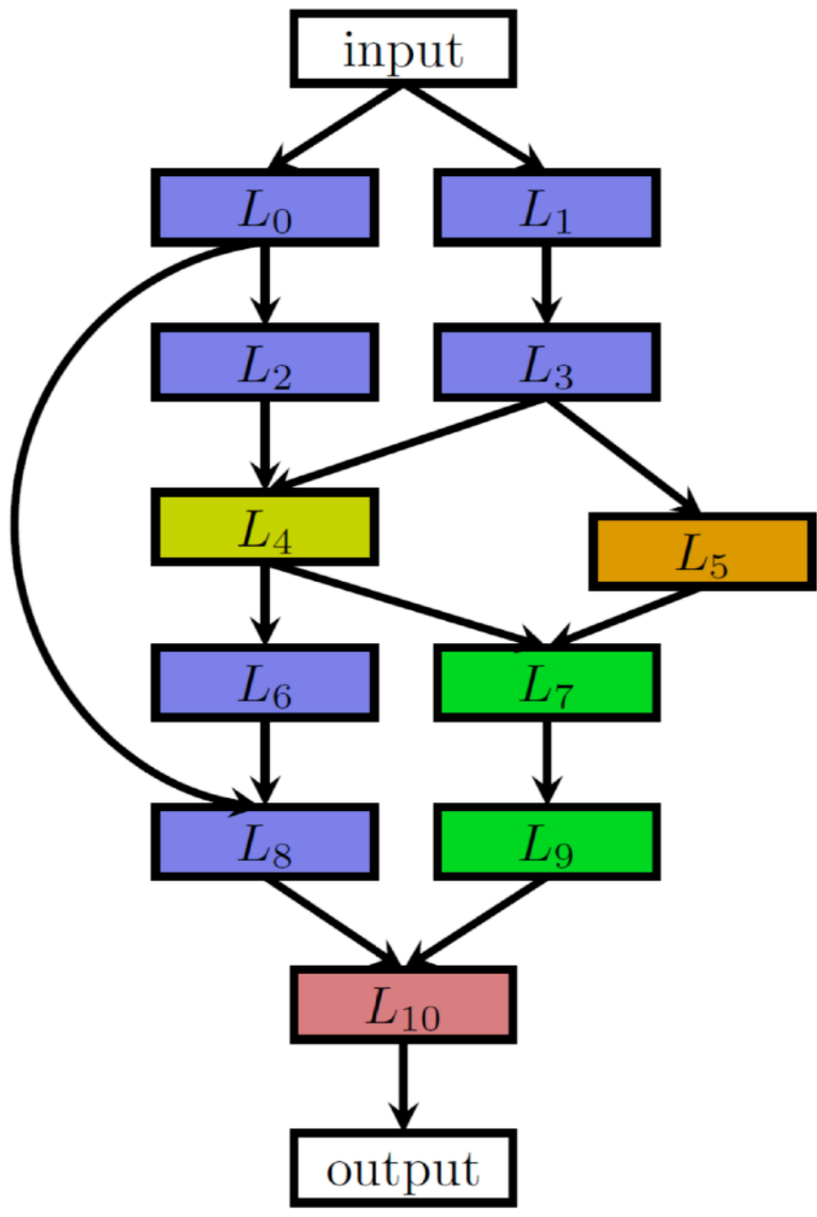
+ easier to search
- sometimes too simple



Parameterized Graph

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

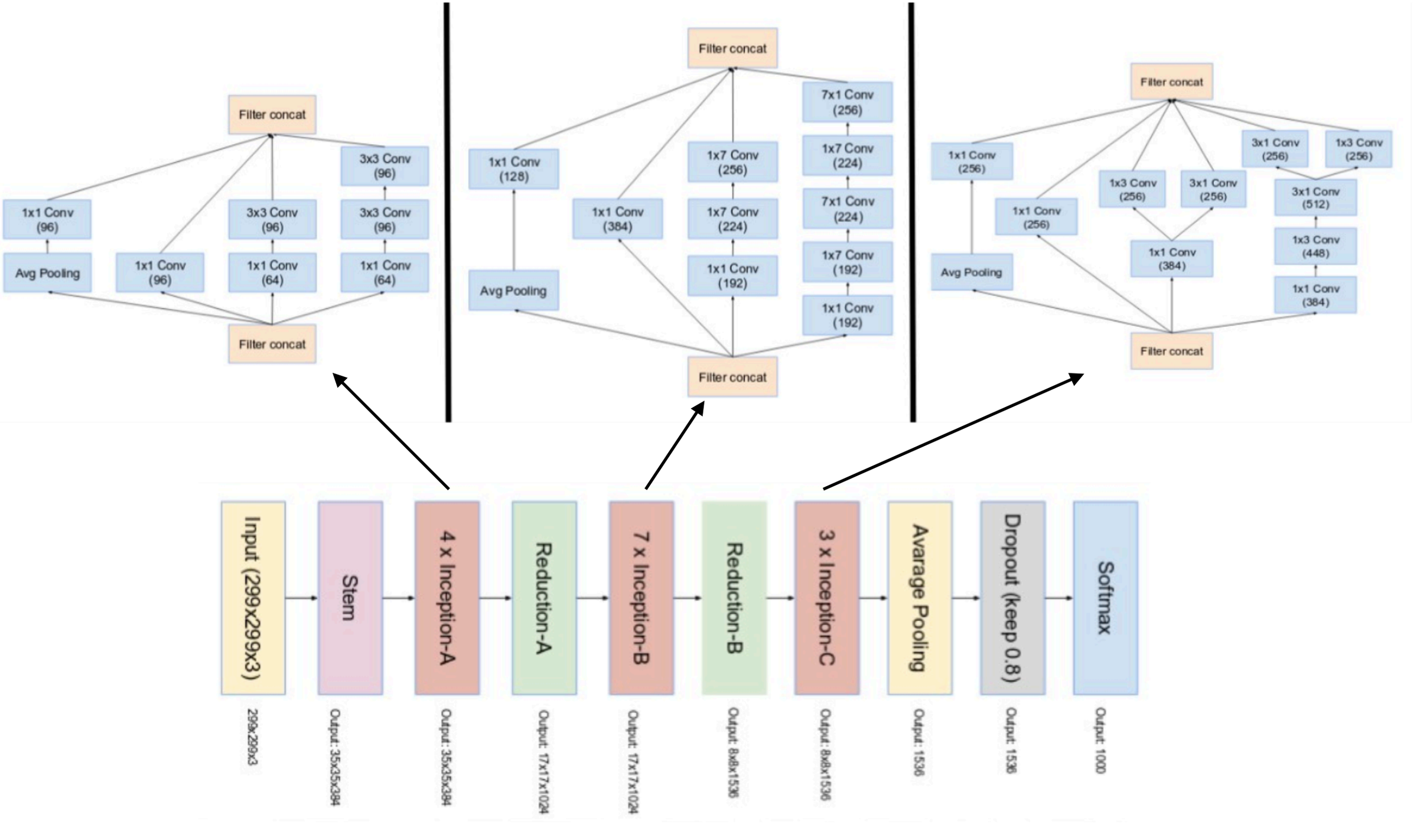
+ more flexible
- much harder to search



Neural Architecture Search

Observation: successful deep networks have repeated motifs (cells)

e.g. Inception v4:



Google NASNet Zoph et al 2018

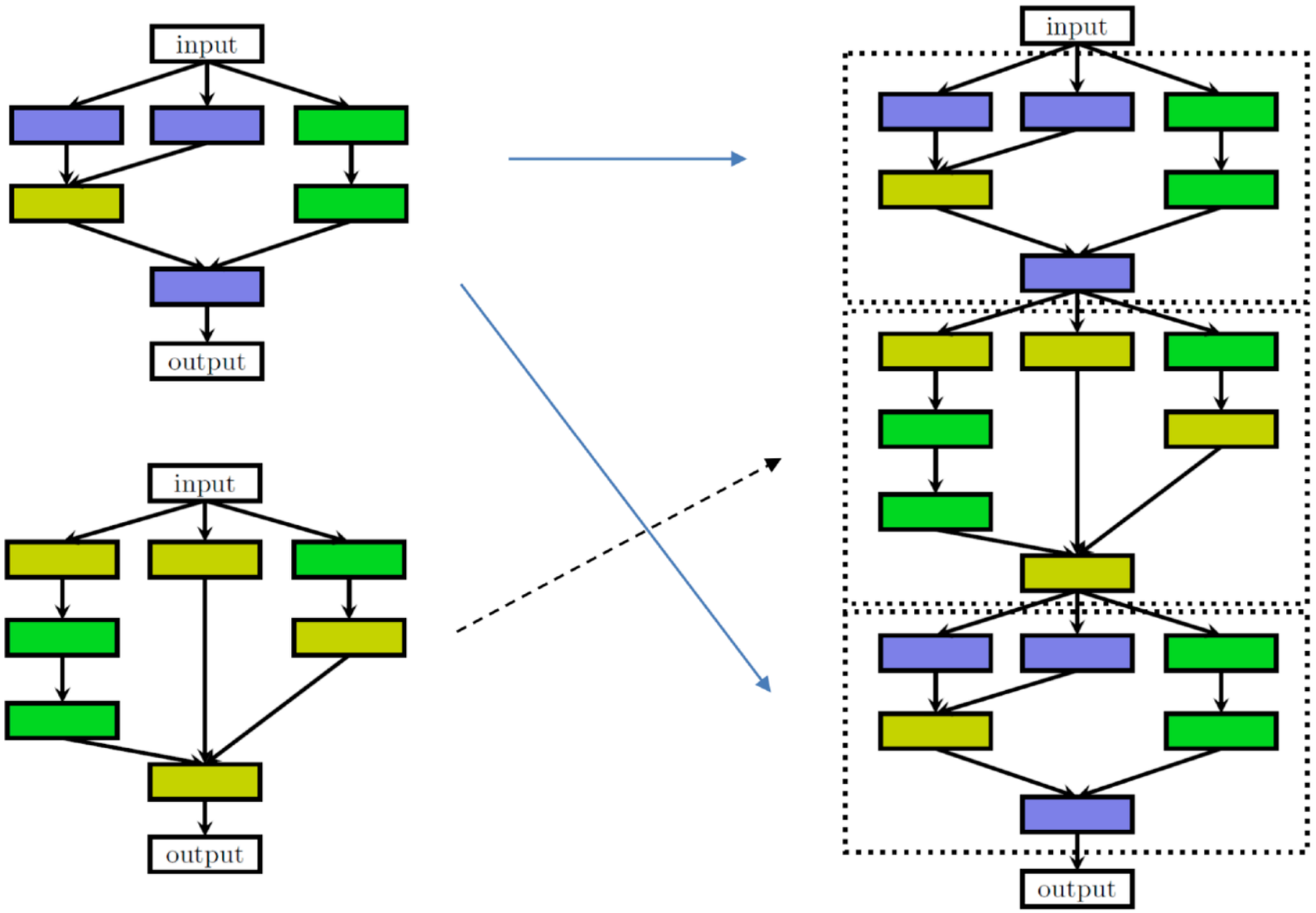
Neural Architecture Search

Observation: successful deep networks have repeated motifs (cells) -> transfer!

Cell search space

- parameterized building blocks *(cells)*

- stack cells together in macro-architecture
  - usually a chain



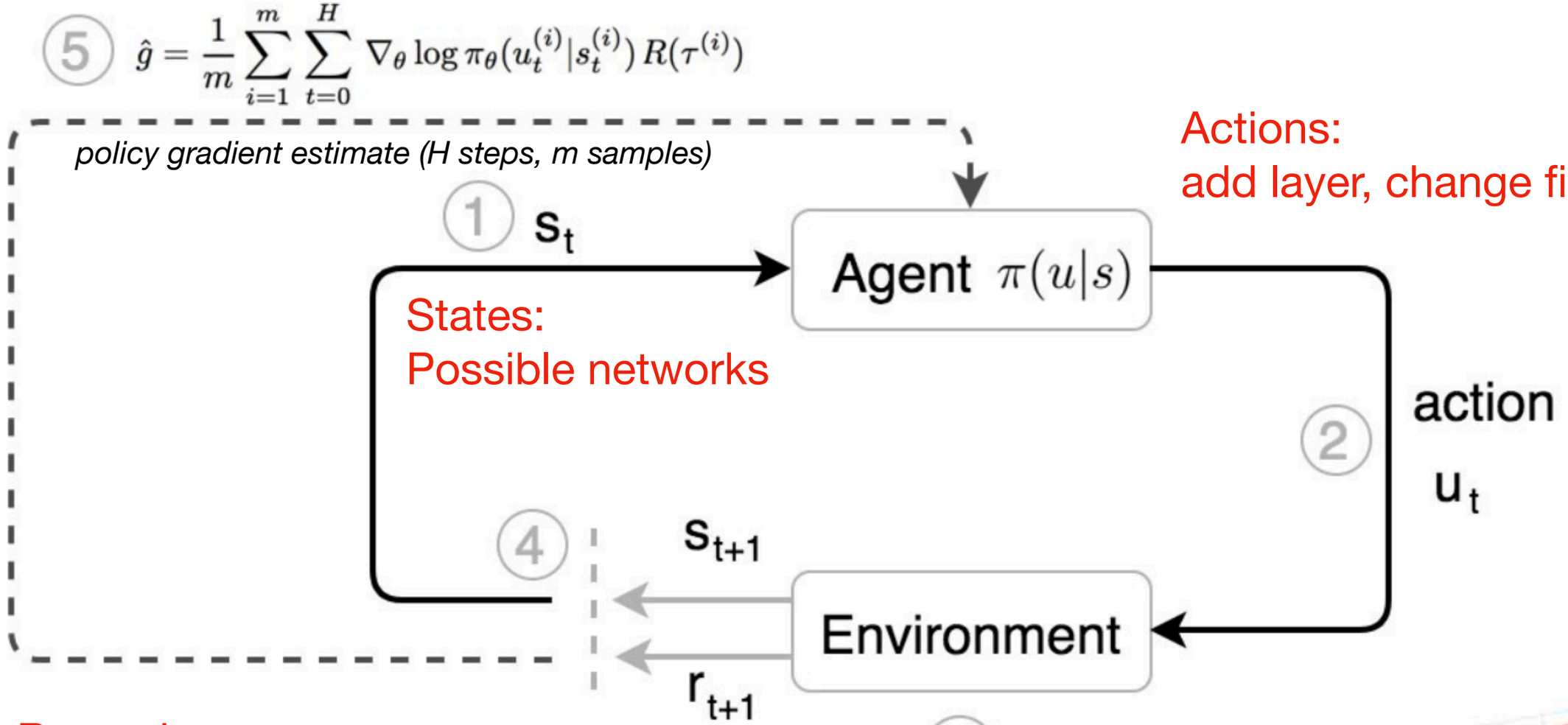
+ smaller search space
+ cells can be learned on a small dataset & transferred to a larger dataset
- you can't learn entirely new architectures

Zoph & Le 2017

Levine Hui

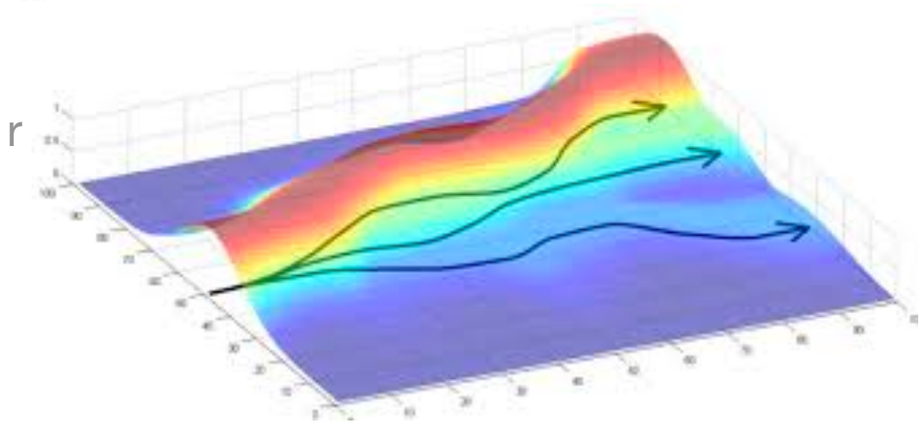
NAS with Reinforcement learning

Build network step-by-step, learn general strategy (policy)



Reward:
Network performance after training

After trajectory τ of actions, adjust policy based on total reward R(τ)

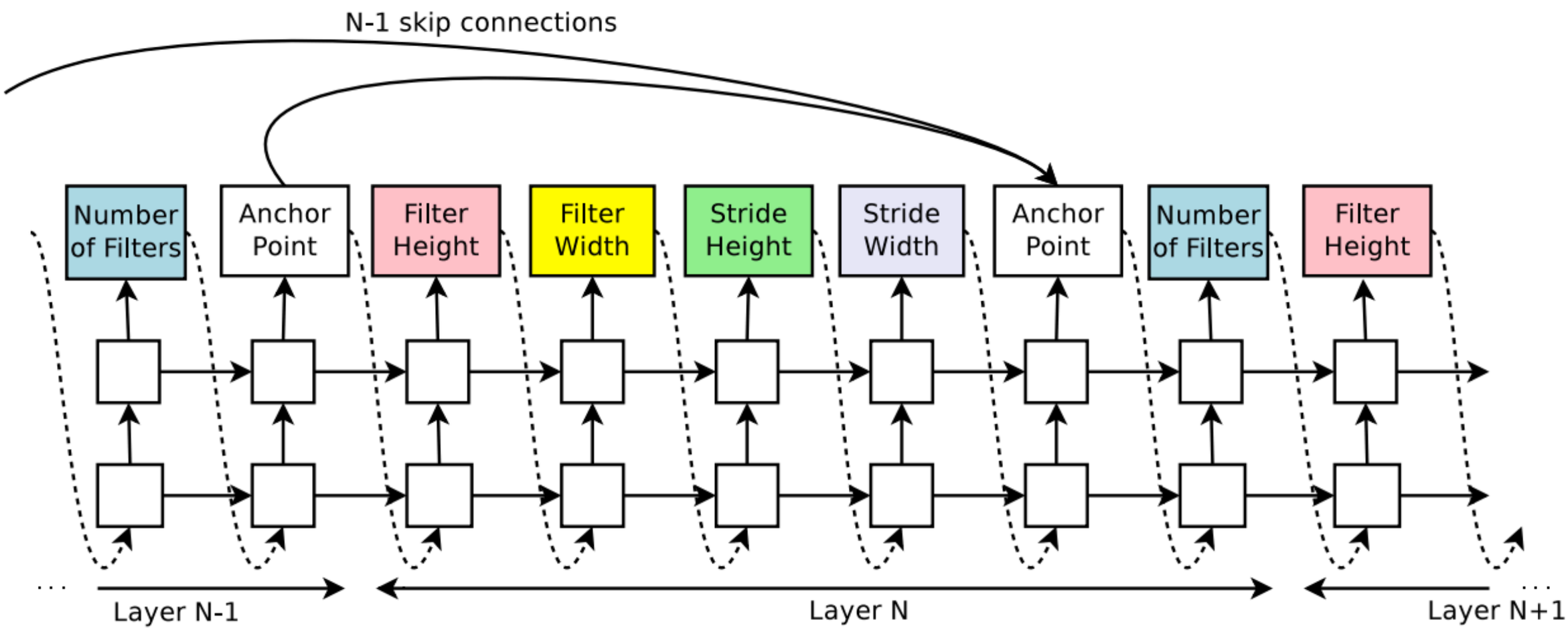


Zoph & Le 2017

NAS with Reinforcement learning

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



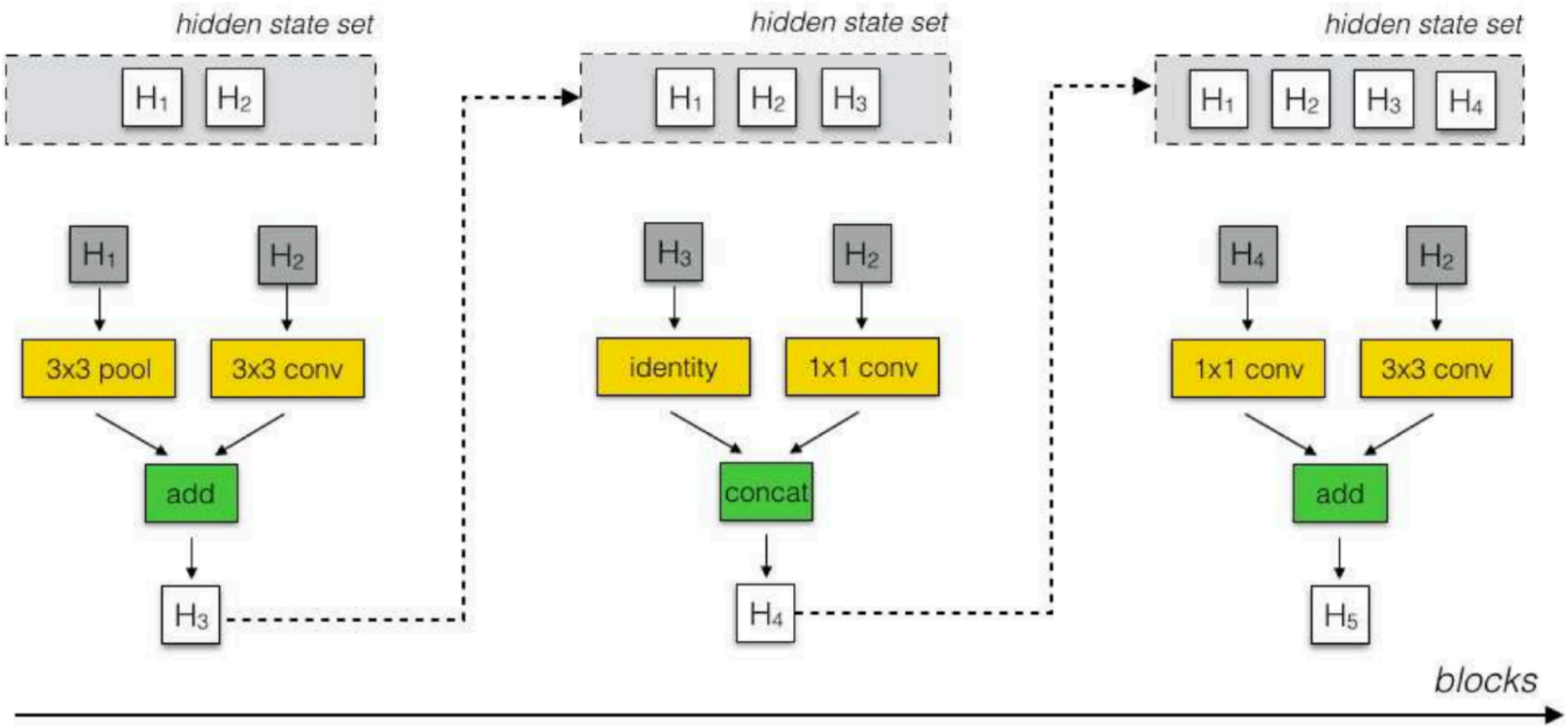
Zoph et al 2018

NAS with Reinforcement learning

1-layer LSTM (PPO), cell space search

- State of the art on ImageNet
- 450 GPUs, 1 week, 20000 architectures

- Cell construction:
  - Select existing layers (hidden states, e.g. cell input) H_i to build on
  - Add operation (e.g. 3x3conv) on H_i
  - Combine into new hidden state (e.g. concat, add,…)
  - Iterate over *B* blocks



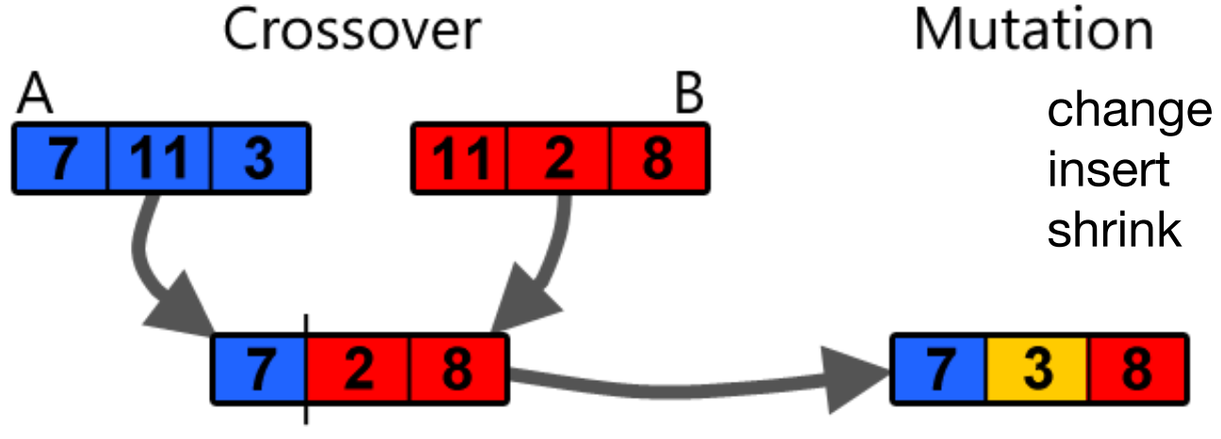
Neuro-evolution

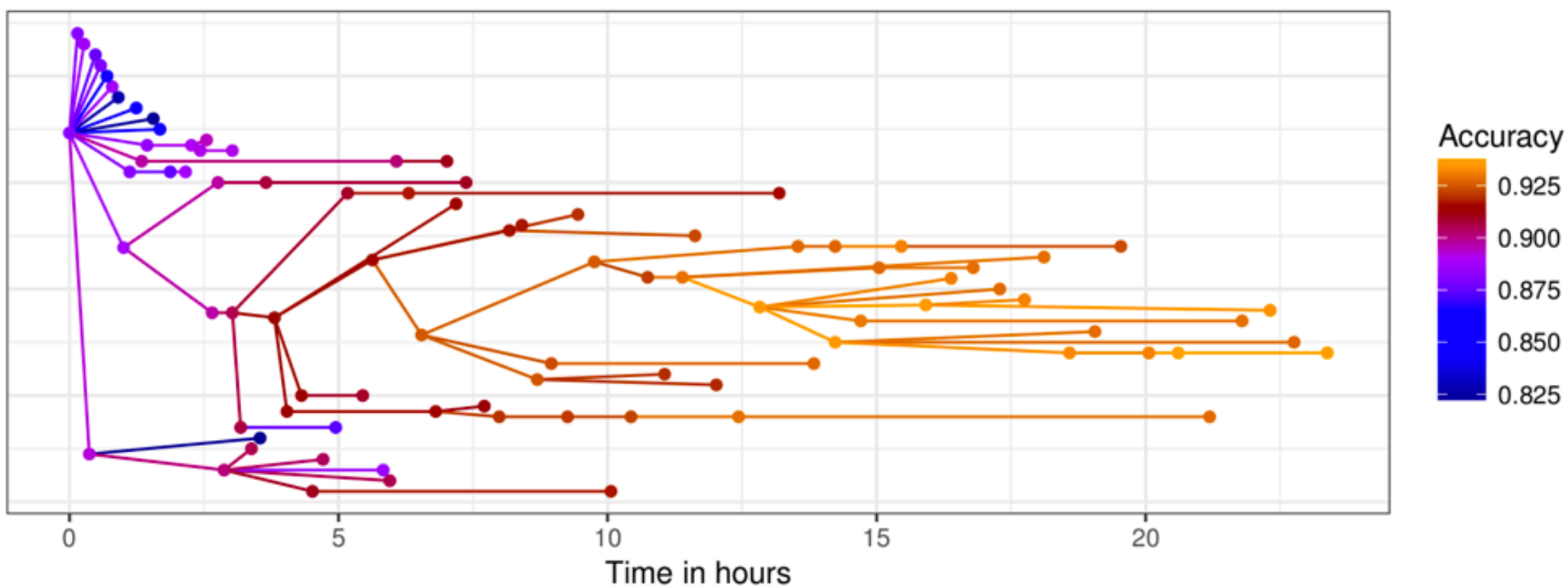
Real et al 2017
Miikkulainen et al 2017
Wistuba et al 2018

- Start with initial architecture
- Best architectures *evolve*: cross-over or mutation
- No fixed maximal length

+ more flexible

- larger search space, can be slower



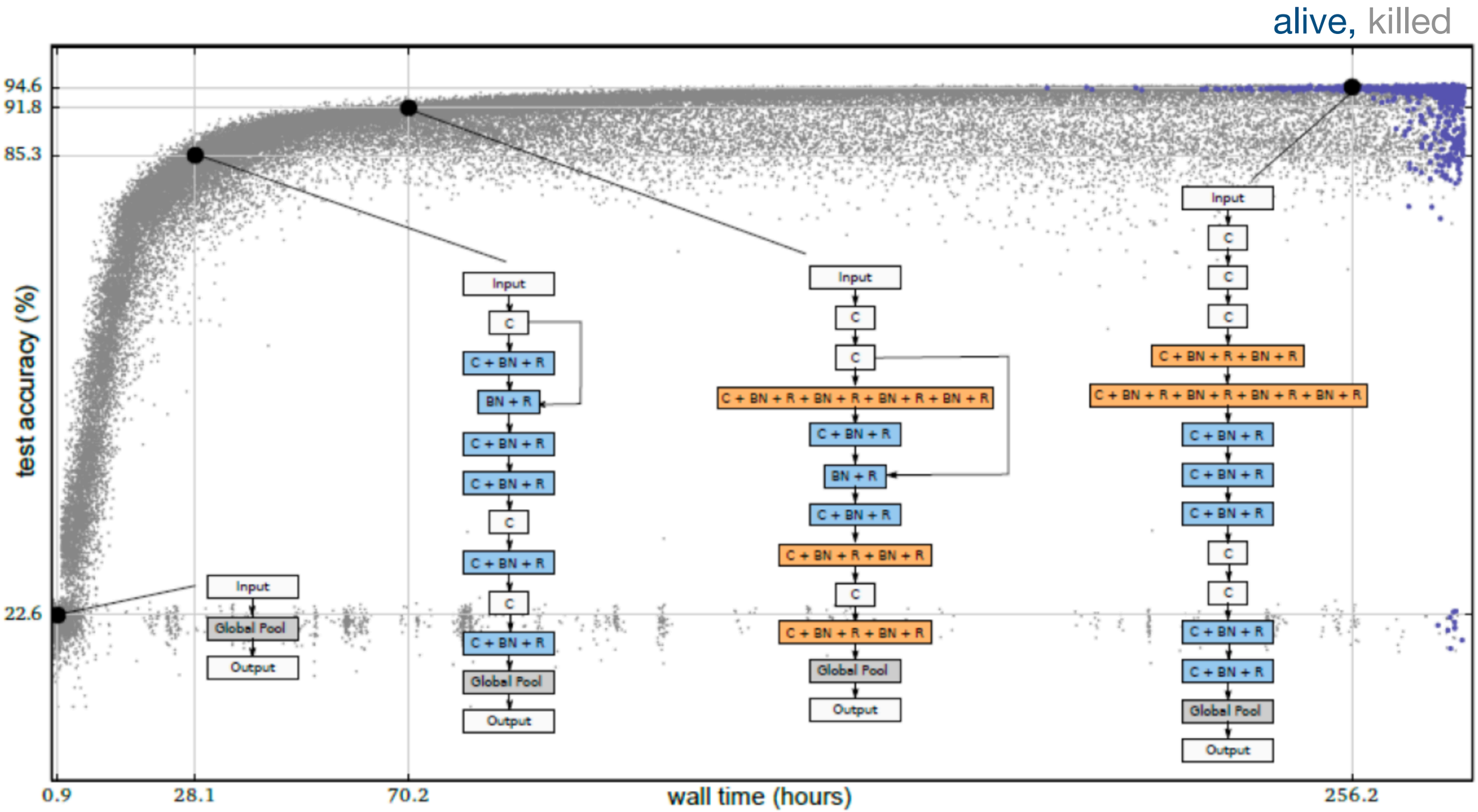


Architecture Search

Neuro-evolution

Real et al 2017
Miikkulainen et al 2017
Wistuba et al 2018

- same idea: learn the neural architecture through evolution
- mutations: add, change, remove layer

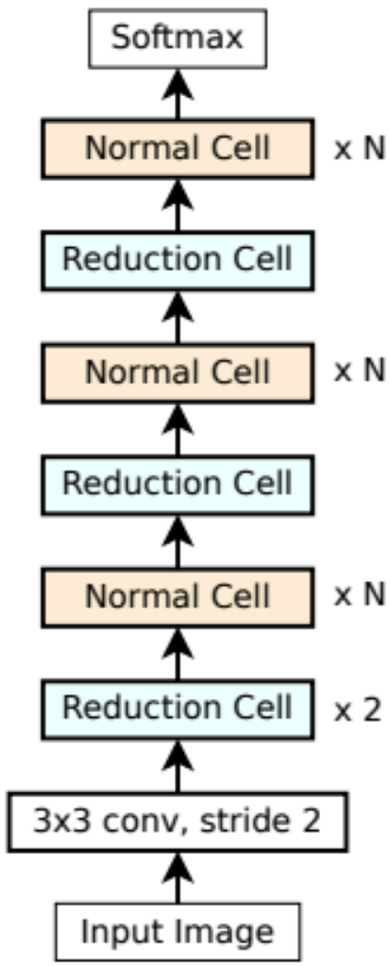


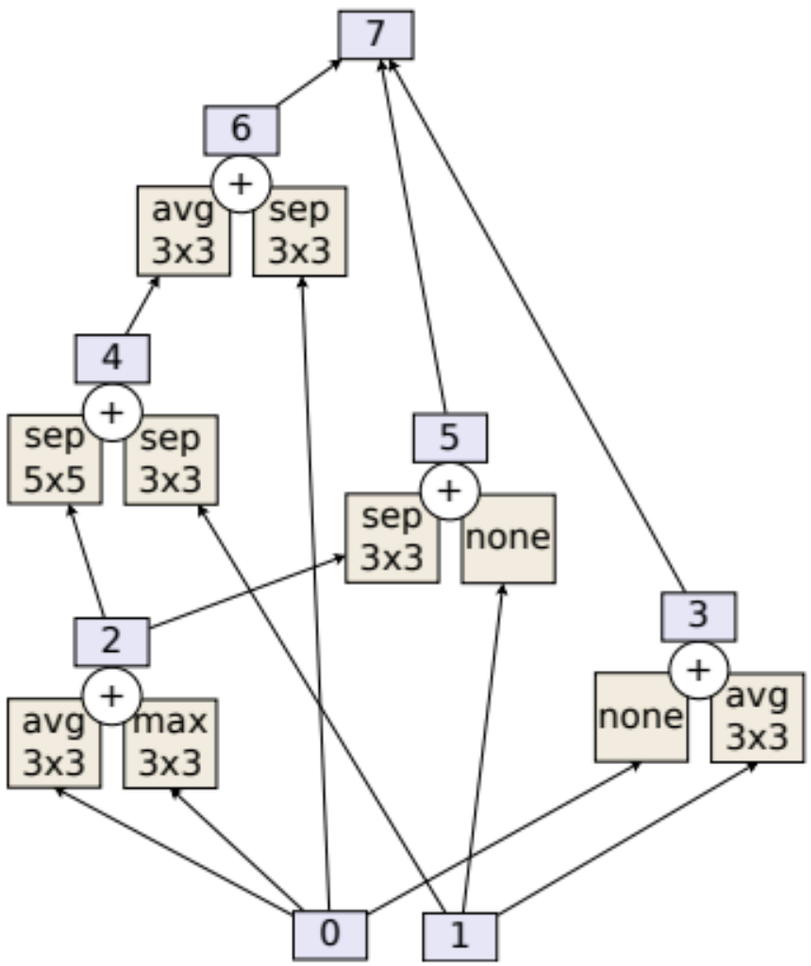
Real et al 2019

Neuro-evolution

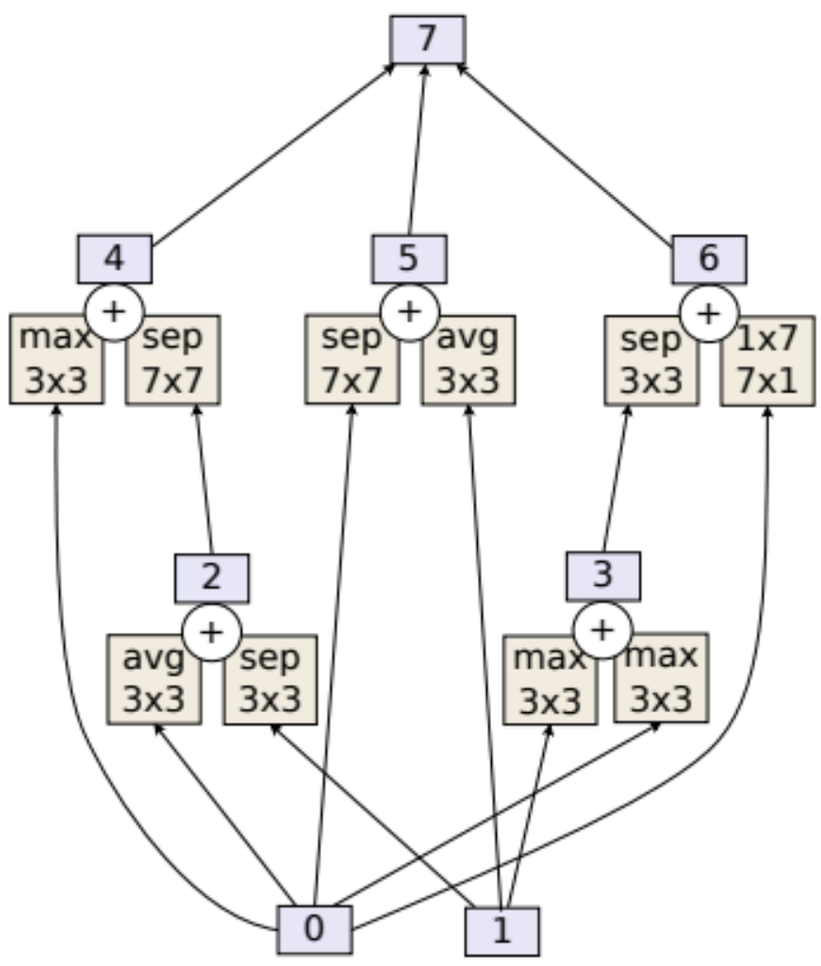
AmoebaNet: State of the art on ImageNet, CIFAR-10

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





normal cell



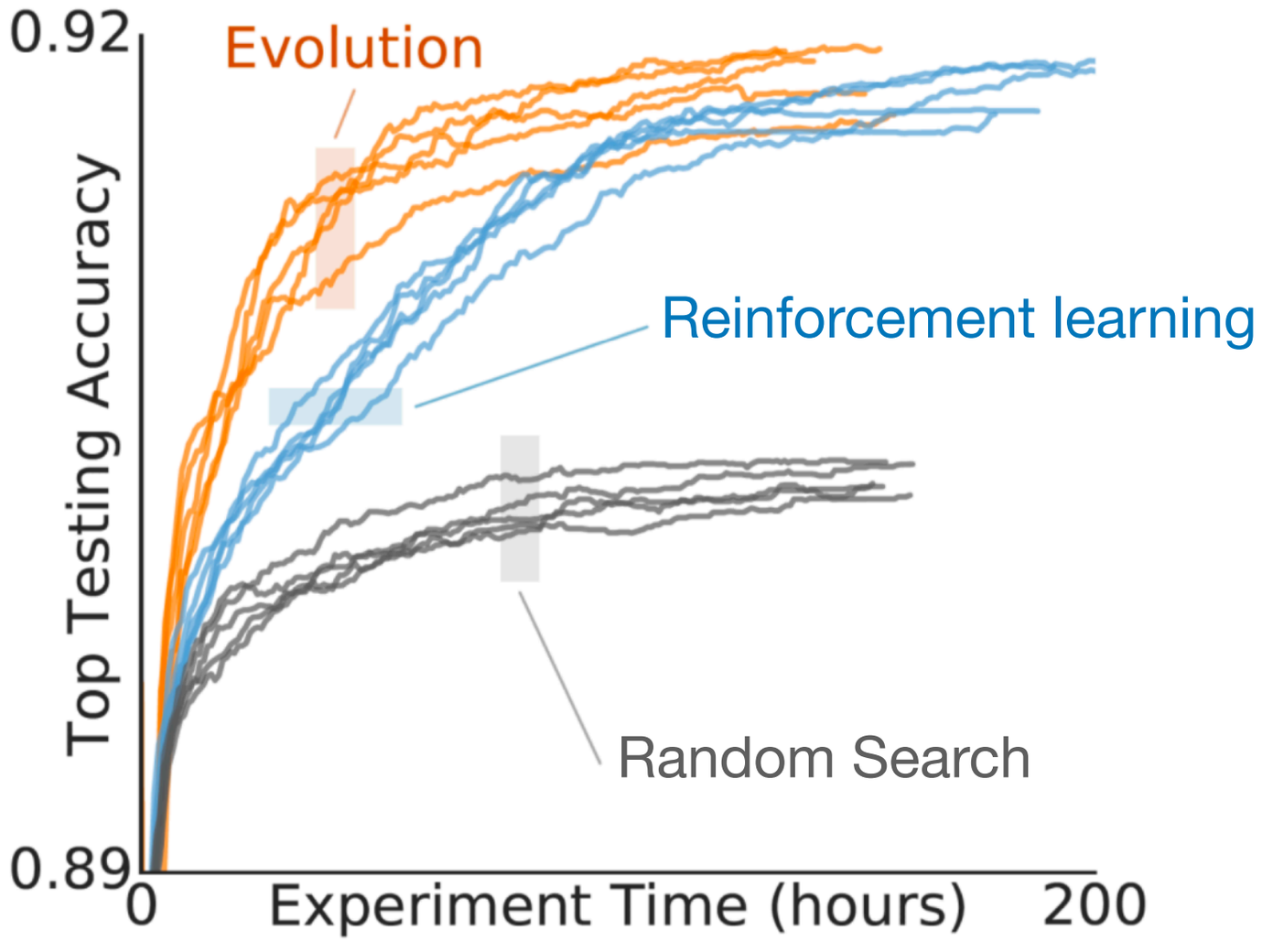
reduction cell

Real et al 2019

Neuro-evolution

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

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

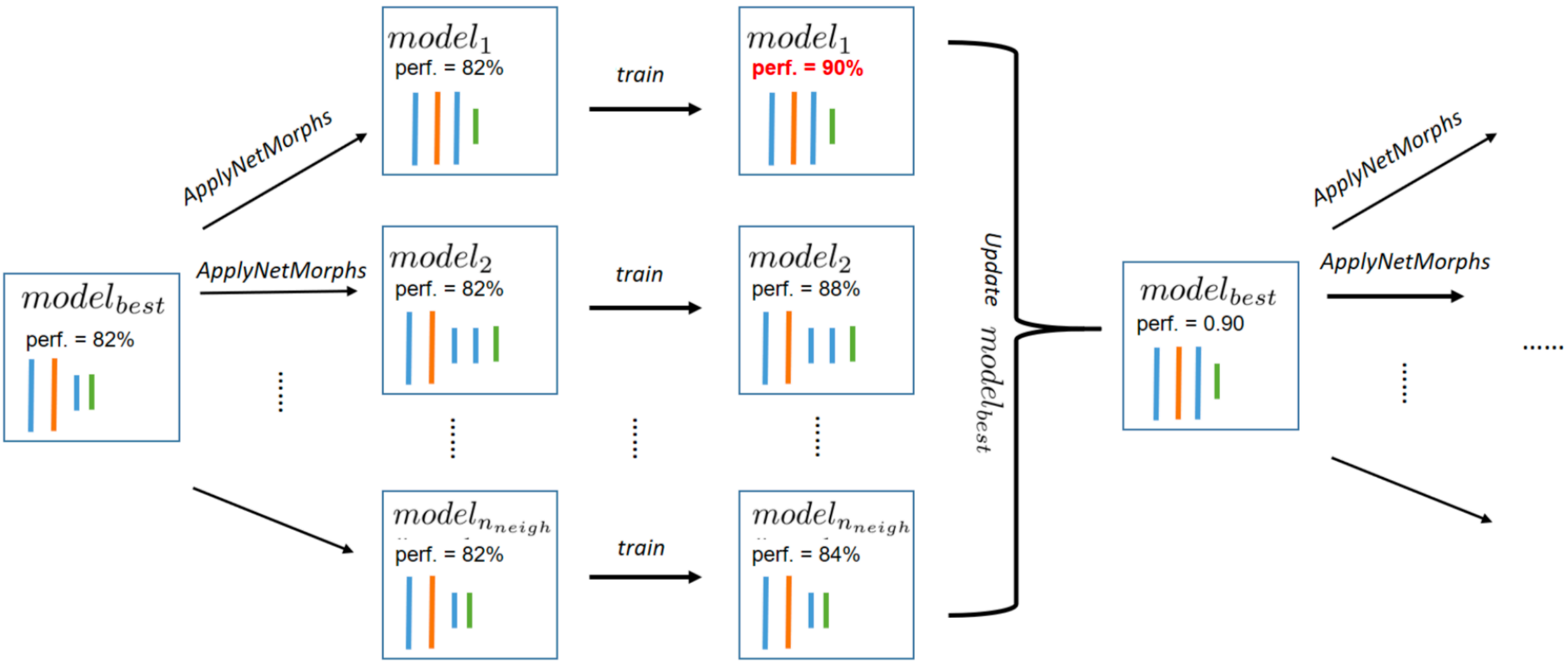


Chen et al. 2016, Wei et al. 2016, Cai et al. 2017
Cai et al. 2018, Elsken et al. 2017, Cortes et al. 2017, Cai et al. 2018

Network Morphisms

[AutoKeras]

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

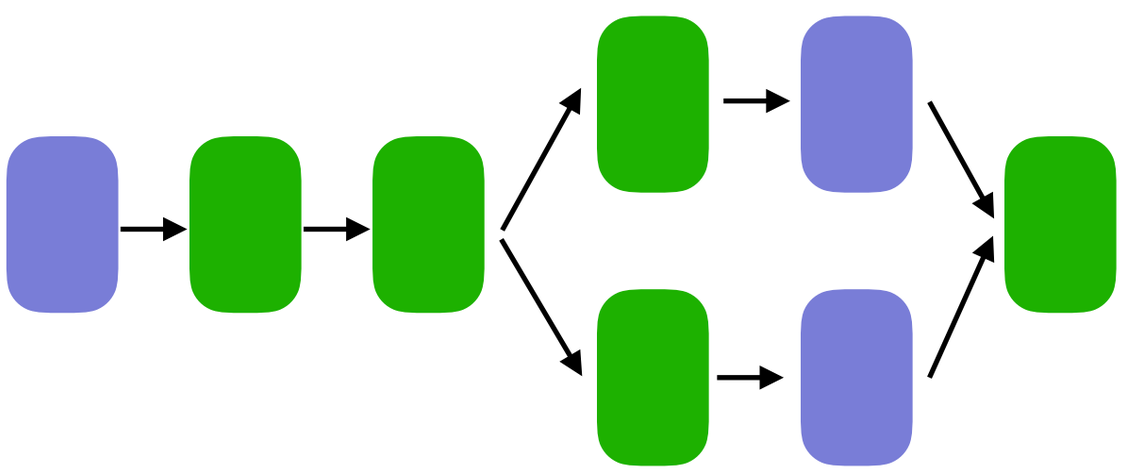


Hyperparameter Optimization

Searching the hyperparameter space ***efficiently***

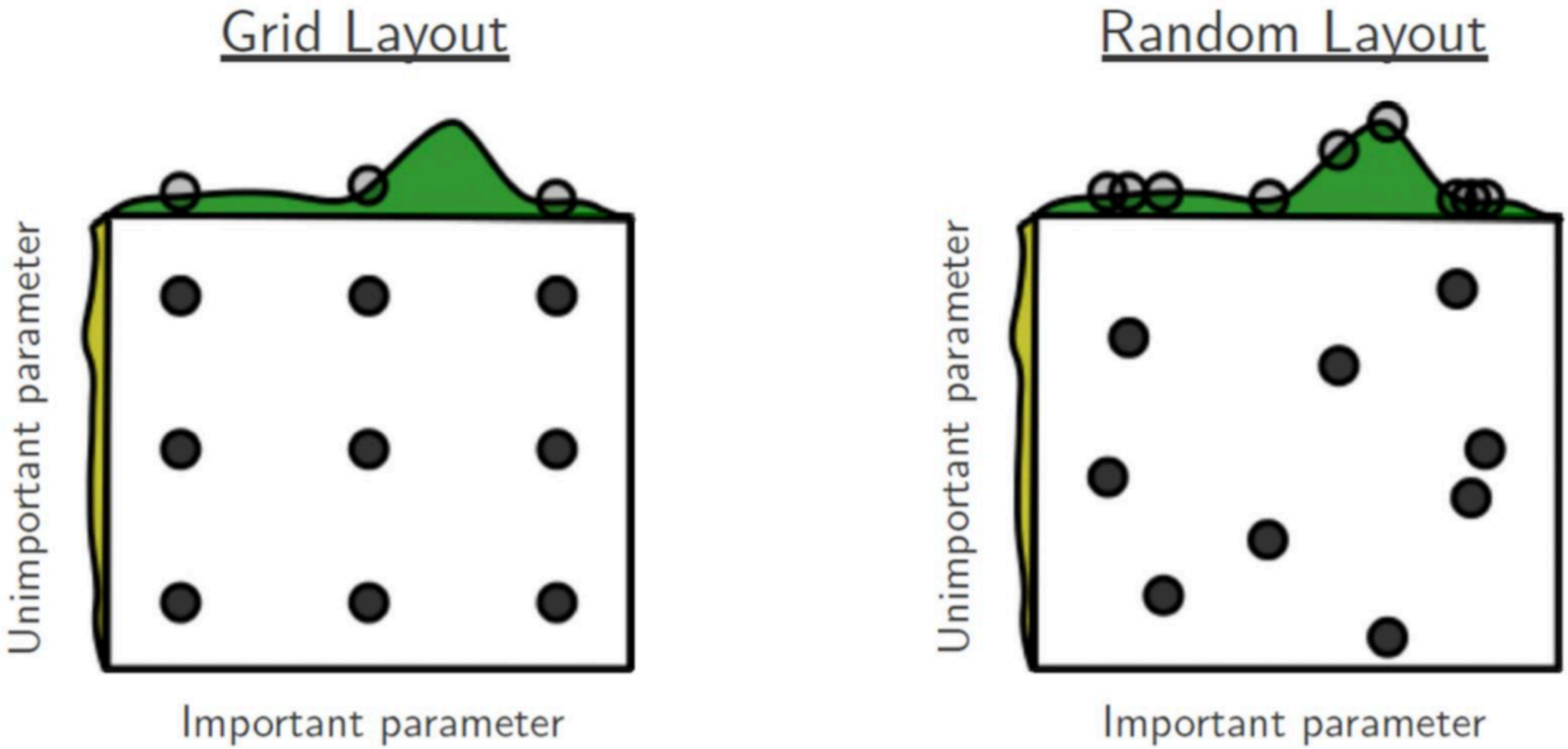
AutoML: subproblems

- **Hyperparameter optimization**: *many different approaches*
  - Random search
  - Bayesian optimization
  - Population-based methods (evolution)
  - Multi-fidelity optimization
  - Differentiable optimization
  - …



Random search

- Handles unimportant dimensions better than grid search
- Easily parallelizable, but uninformed (no learning)

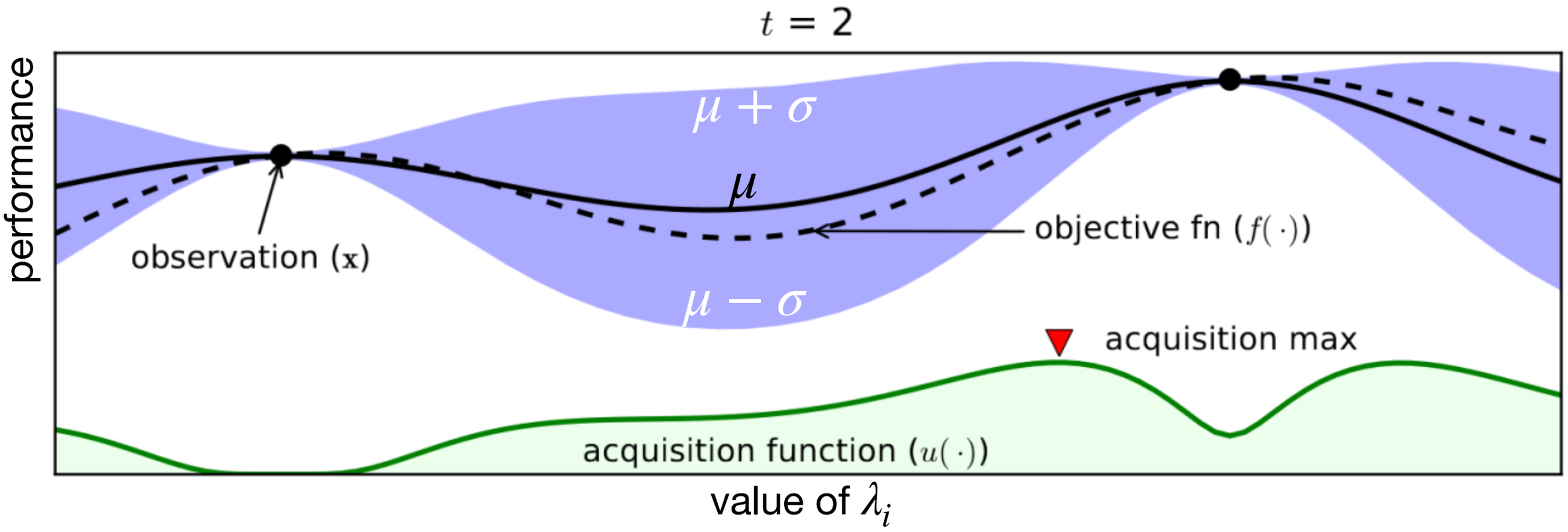


Bergstra & Bengio, JMLR 2012

Mockus [1974]

Bayesian Optimization

- Start with a few (random) hyperparameter configurations
- Fit a ***surrogate model*** to predict other configurations
- Probabilistic regression: mean μ and standard deviation σ (blue band)
- Use an ***acquisition function*** to trade off exploration and exploitation, e.g. Expected Improvement (EI)
- Sample for the best configuration under that function



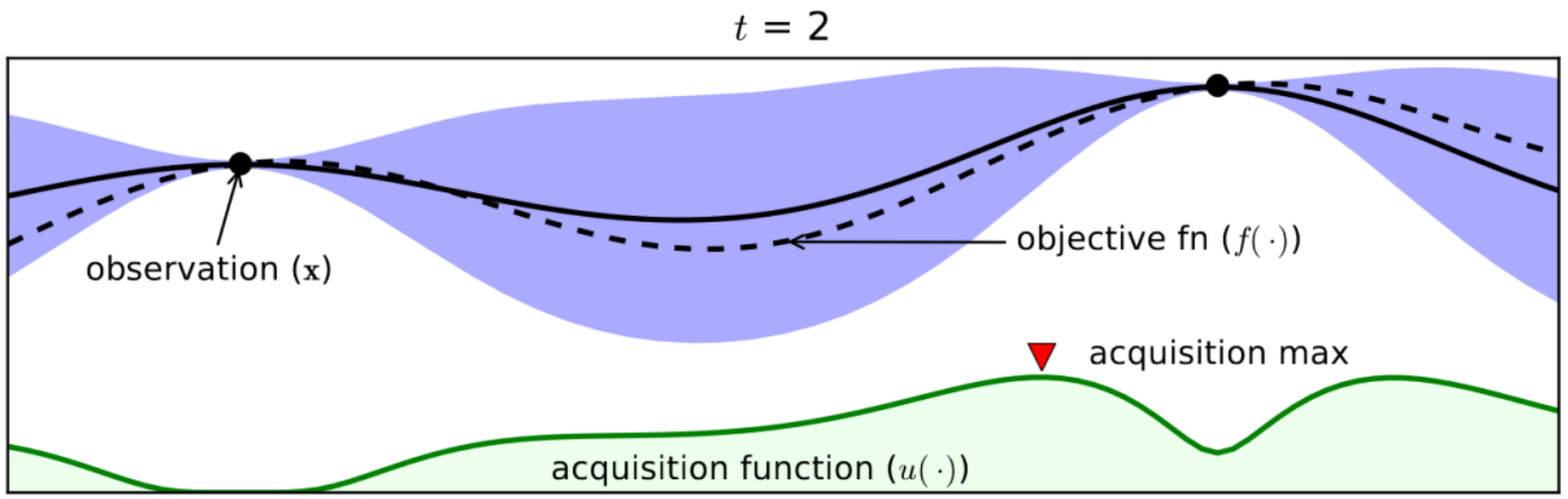
Bayesian Optimization

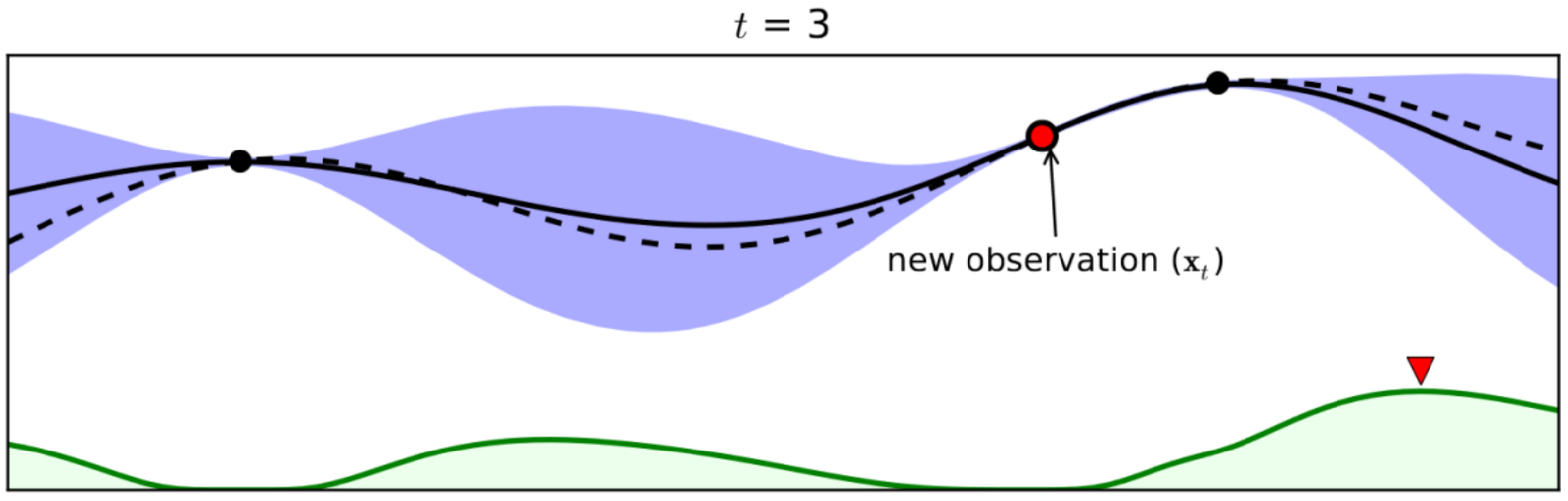
- Repeat until some stopping criterion:
  - Fixed budget
  - Convergence
  - EI threshold

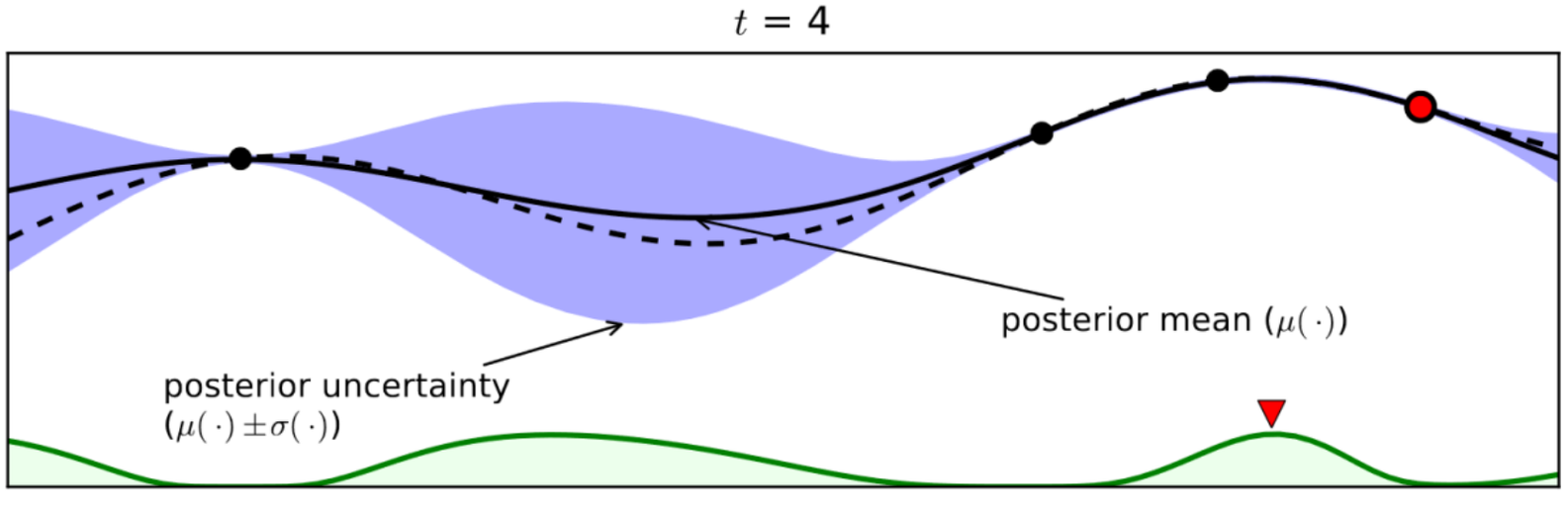
- Theoretical guarantees

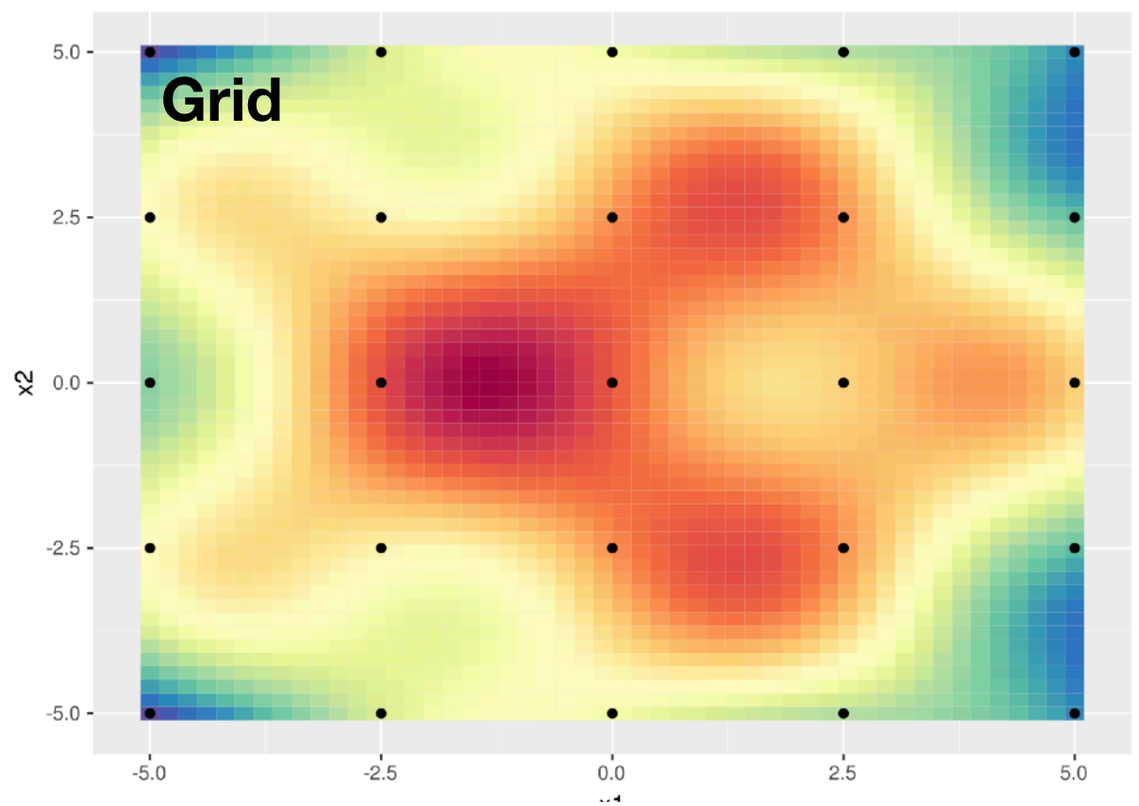
  Srinivas et al. 2010, Freitas et al. 2012, Kawaguchi et al. 2016

- Also works for non-convex, noisy data
- Used in AlphaGo








Grid
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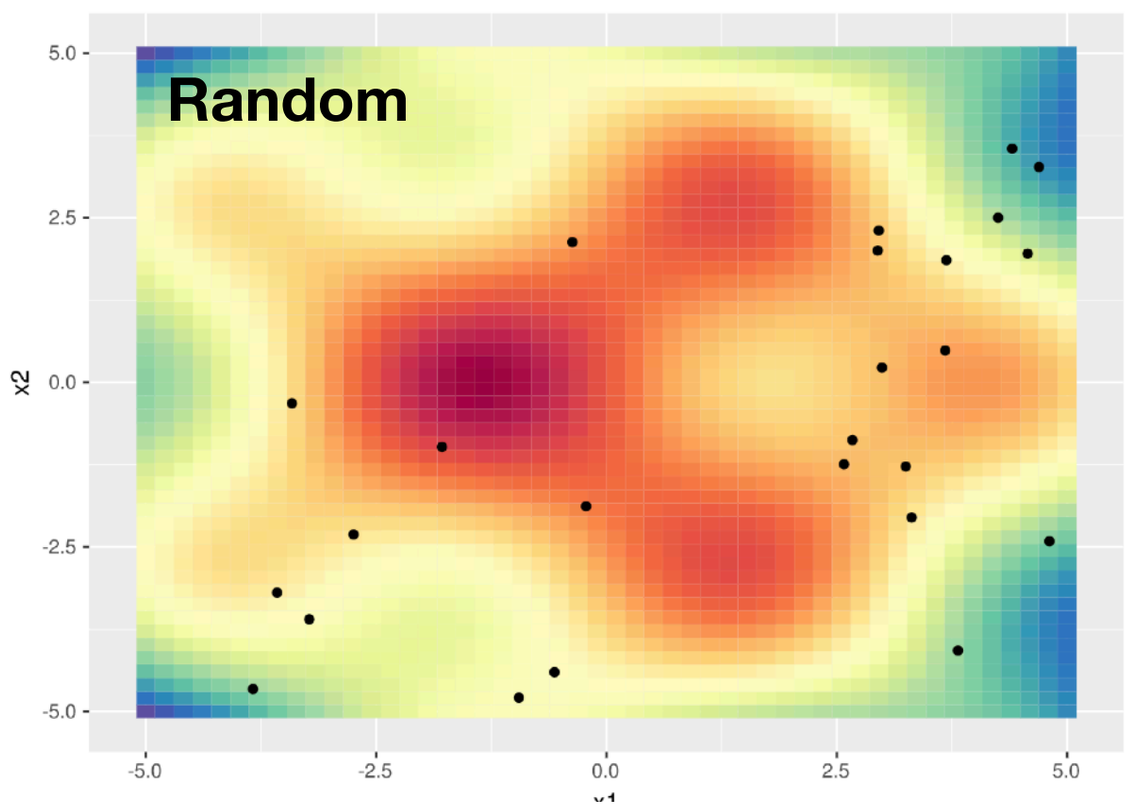
Random
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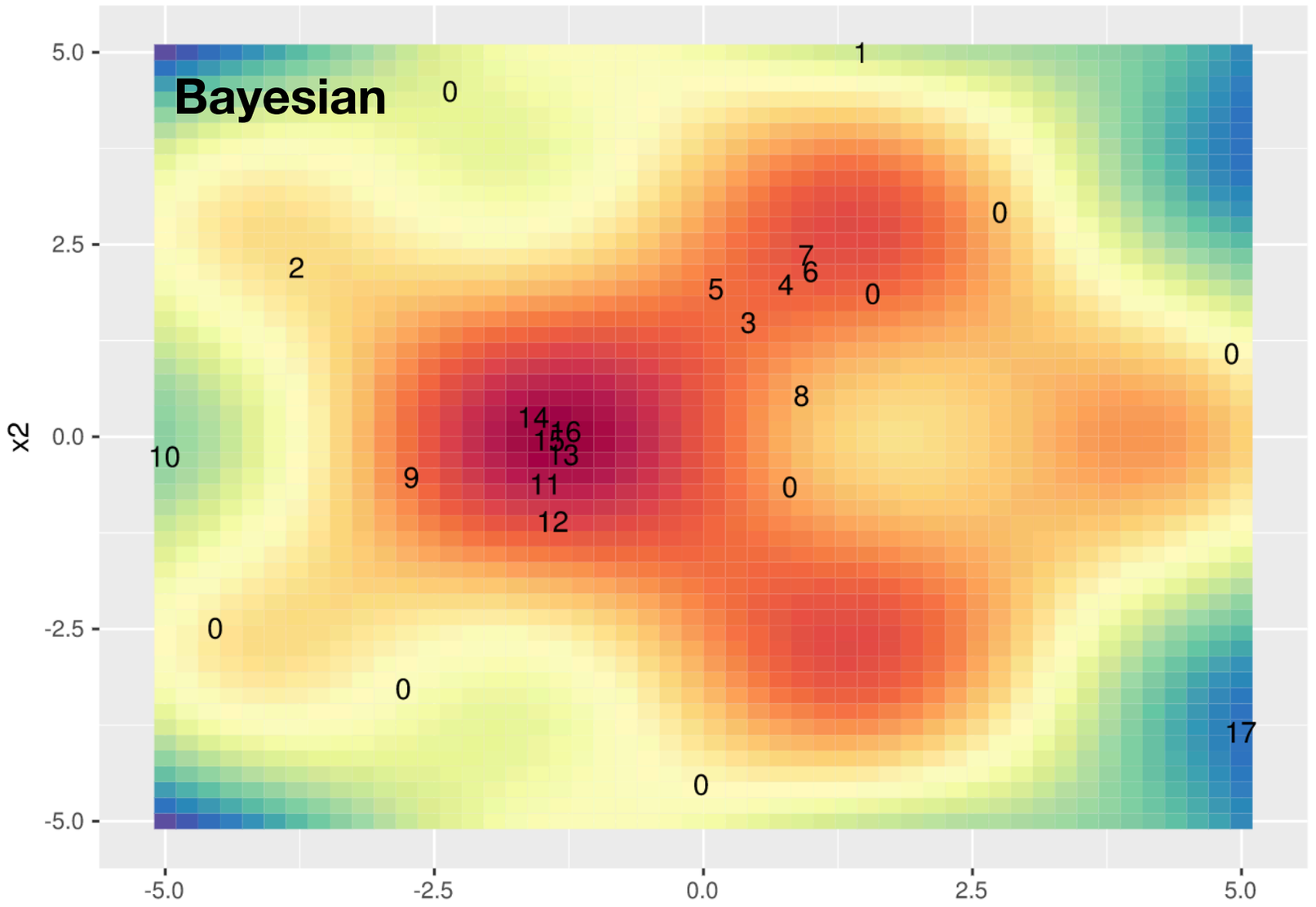
Bayesian
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x2
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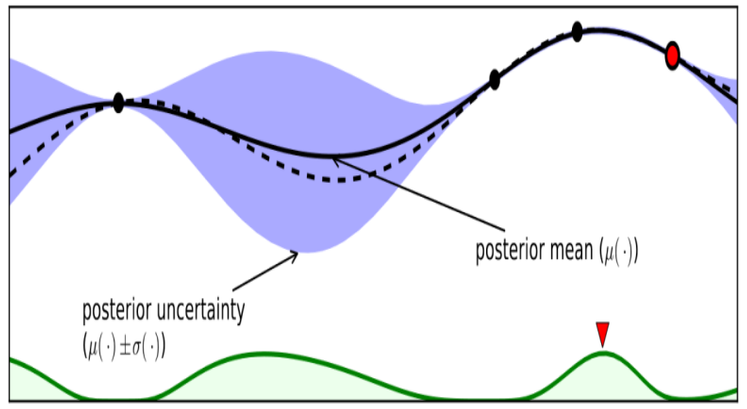
Hyperparameter optimization

Bayesian Optimization: which surrogate?



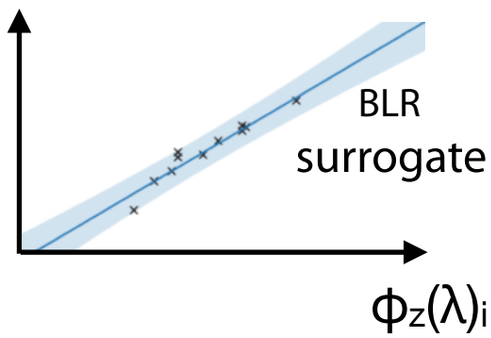
Gaussian processes *[skopt]*

+ handles uncertainty, extrapolates well

+ ideal for few numeric hyperparameters

- scales badly (cubic), try random embeddings *[Wang et al. 2013]*

Bayesian Linear Regression *[Snoek et al. 2015]* *[Amazon AutoML]*



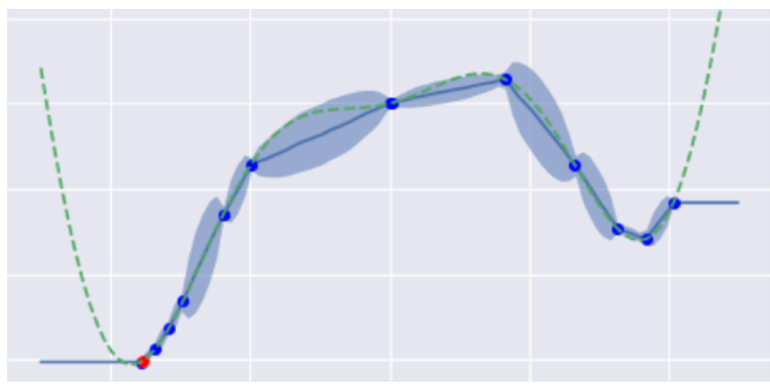
+ Scalable, Bayesian, - requires good basis expansion

Bayesian neural networks *[Springenberg et al. 2016]*

+ Bayesian - Scalability?

[SMAC]

Random Forests *[Hutter et al. 2011, Feurer et al. 2015]*



+ scalable, handles conditional hyperparams

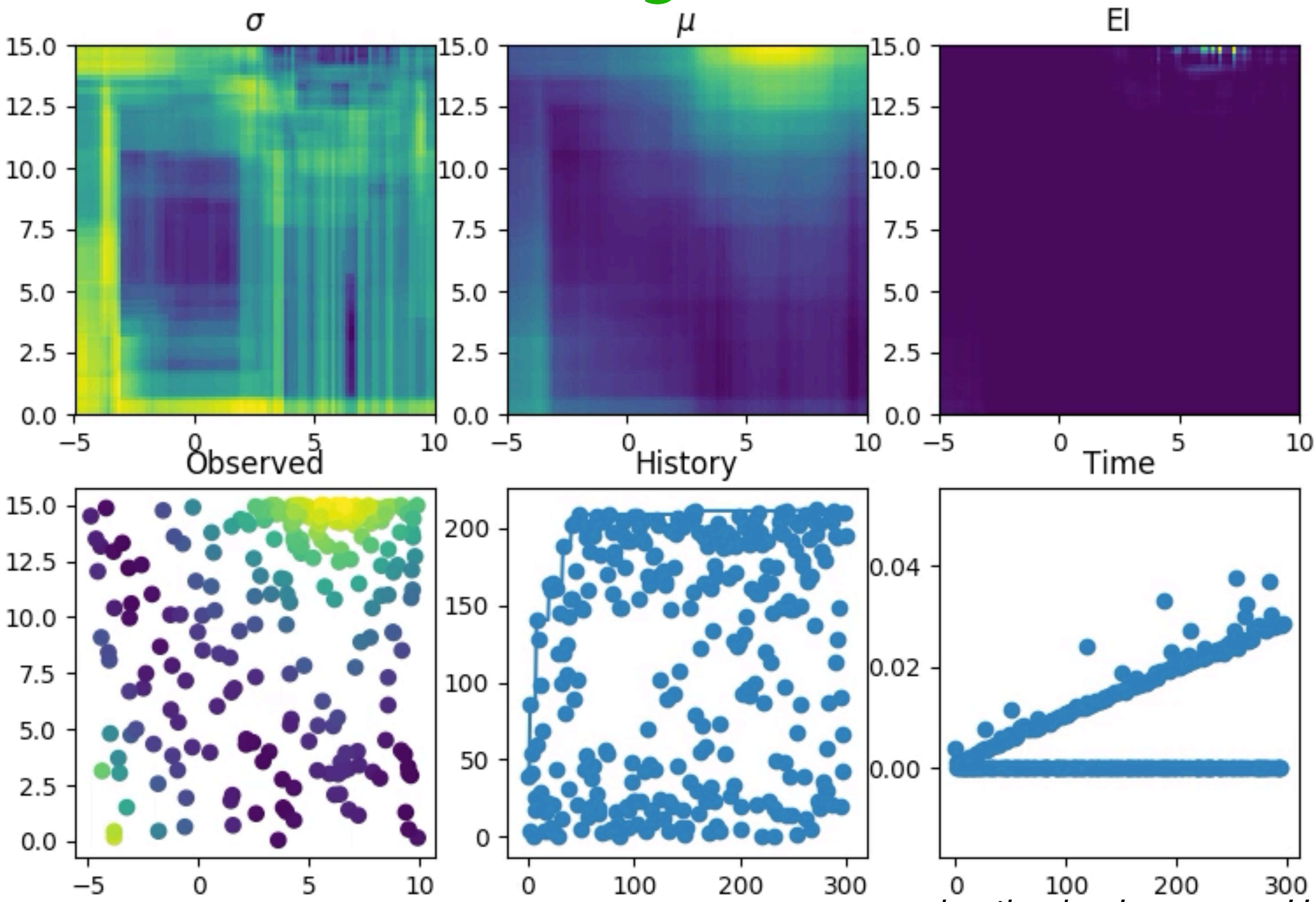
- bad uncertainty estimates, extrapolation

Boosting + quantile regression *[van Hoof, Vanschoren 2019]* *[HyperBoost]*

+ better fit than RF, handles conditionals, adapts to drift - new

Hyperparameter optimization

Random Forest Surrogate



animation by Jeroen van Hoof

[Komer et al. 2019]

Tree of Parzen Estimators

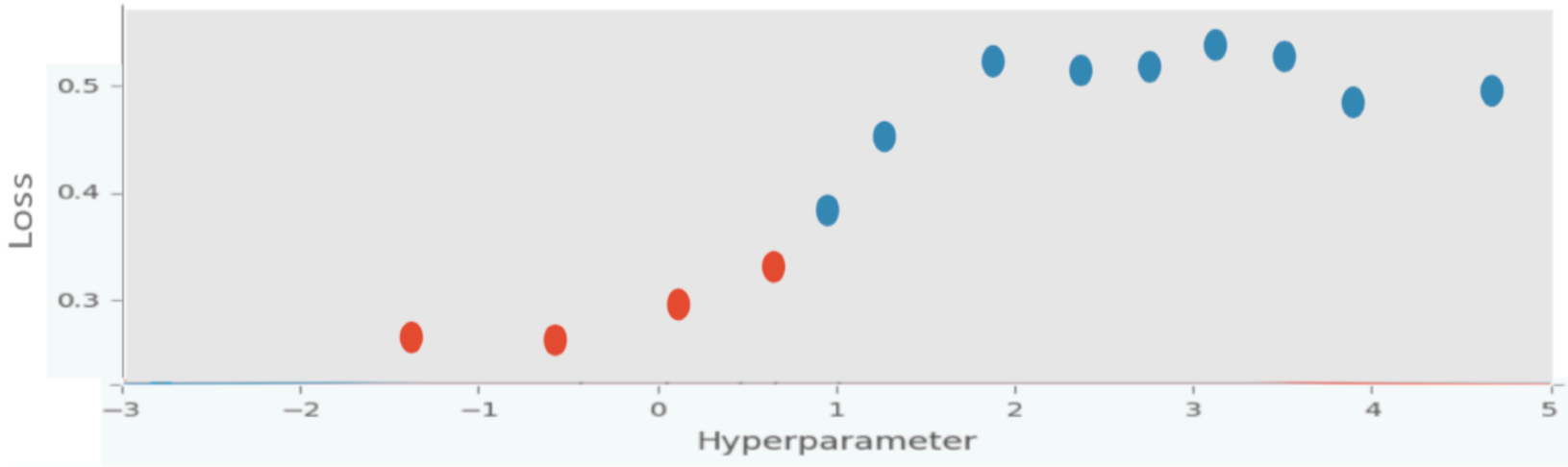
1.Test some hyperparameters

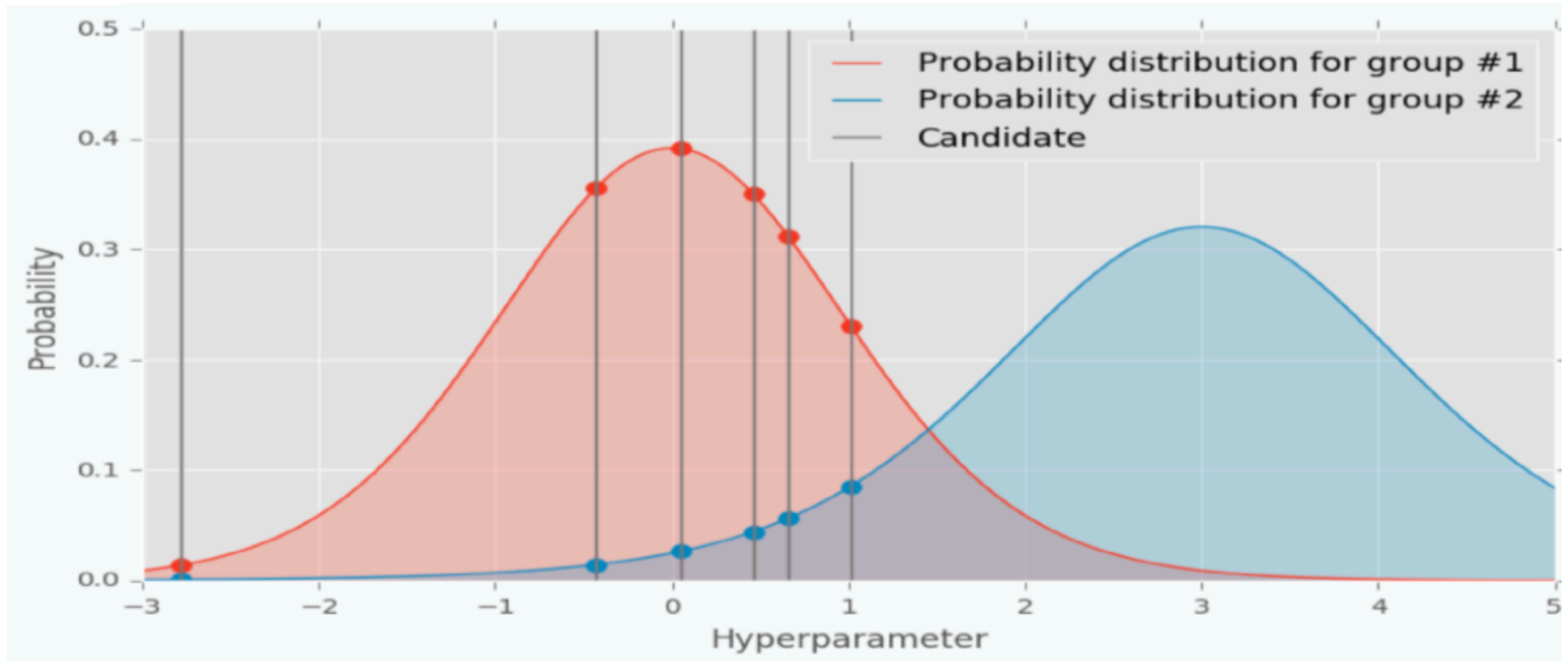
2. Separate into good and bad hyperparameters (with some quantile)

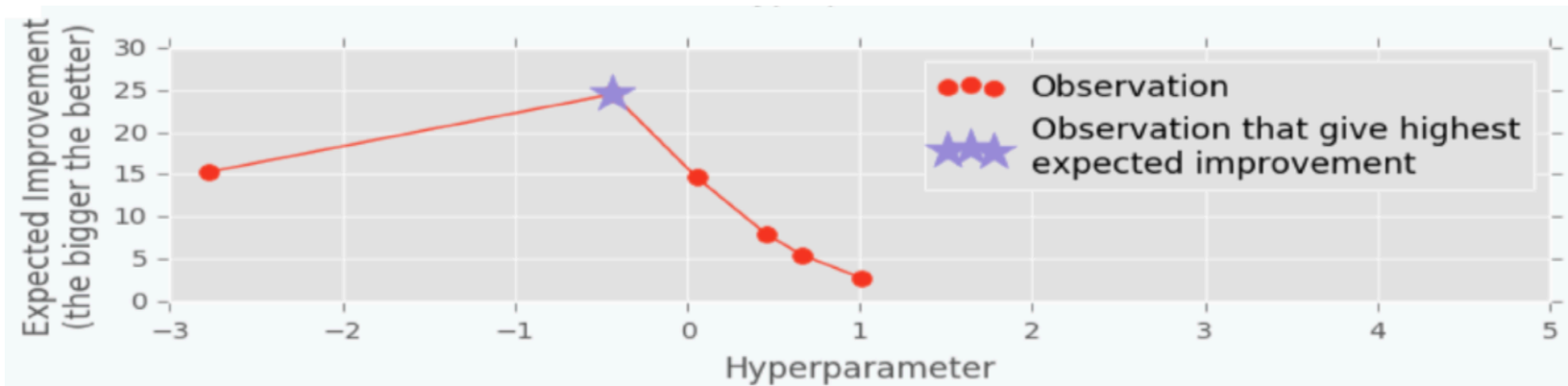
3. Fit non-parametric KDE for $p(\lambda = \text{good})$ and $p(\lambda = \text{bad})$

4. For a few samples, evaluate $\dfrac{p(\lambda = \text{good})}{p(\lambda = \text{bad})}$
Shown to be equivalent to EI!

Efficient, **parallelizable**, robust, but less sample efficient than GPs





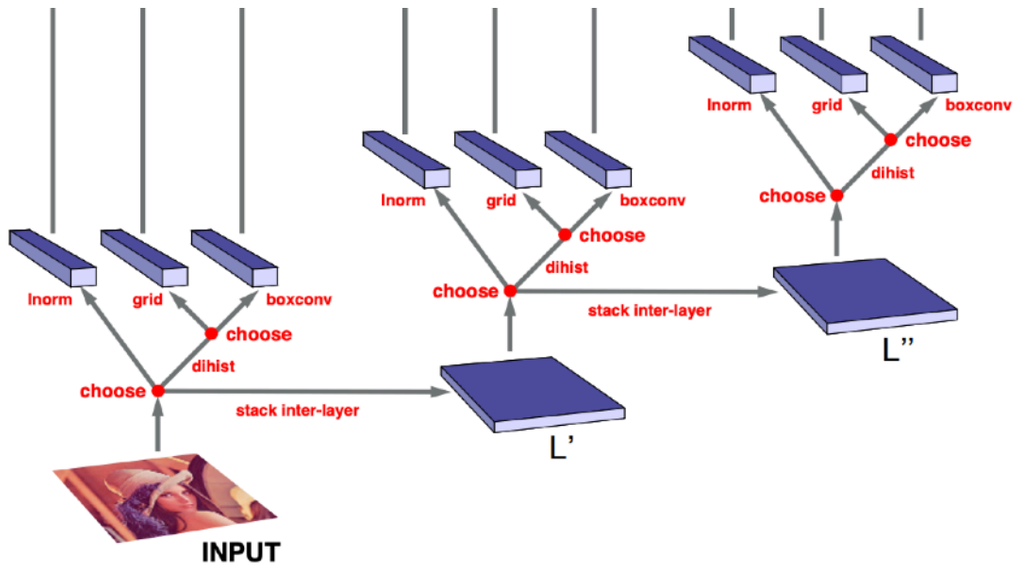


Bayesian Optimization

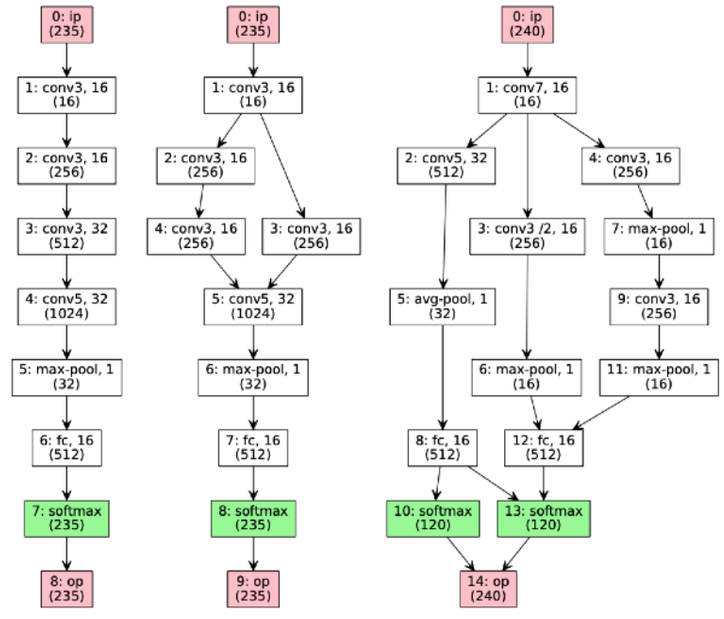
[1] Bergstra et al. 2013
[2] Swersky et al 2013
[3] Kandasamy et al. 2018

Examples:

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



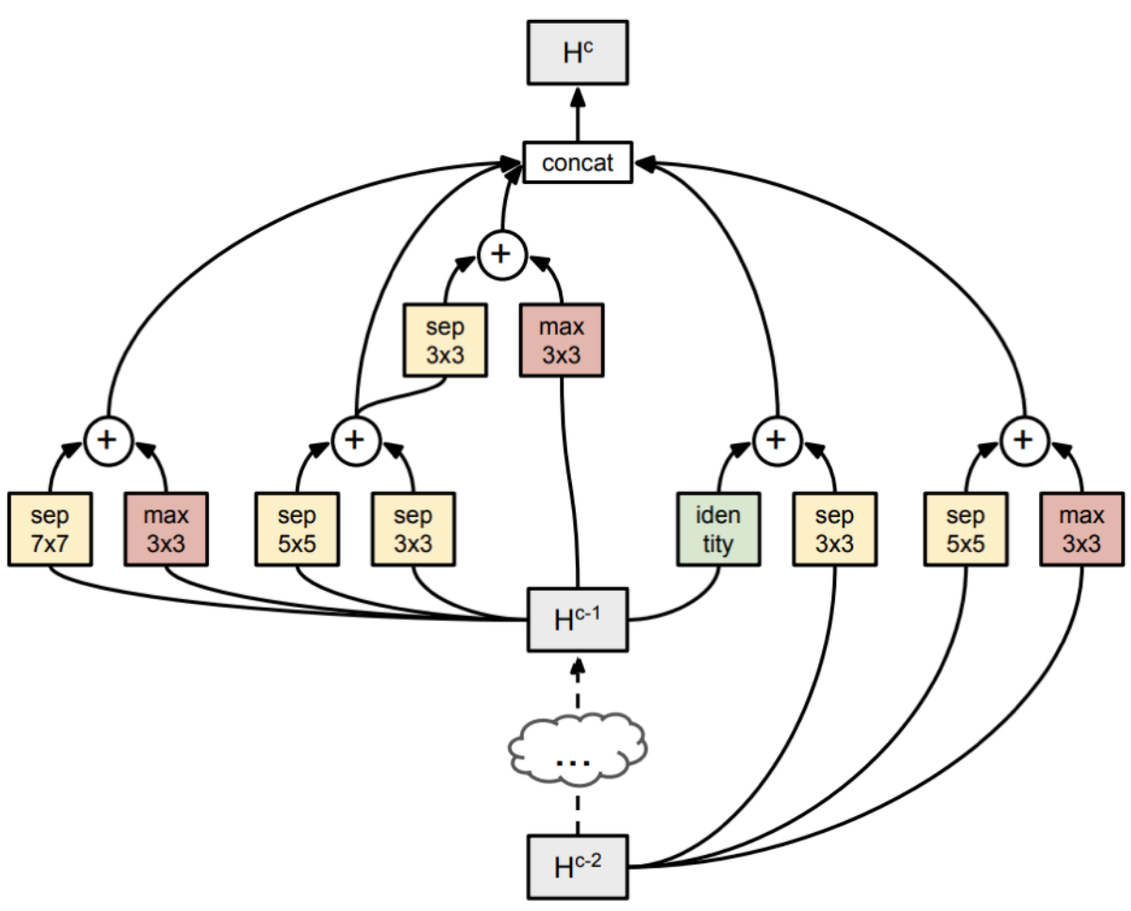
- Kernels to optimize neural nets with GP-based Bayesian optimization
  - ArcNet[2]: DNNs, 23 hyperparameters, 6 kernels
  - NASBOT[3]: DNNs and CNNs

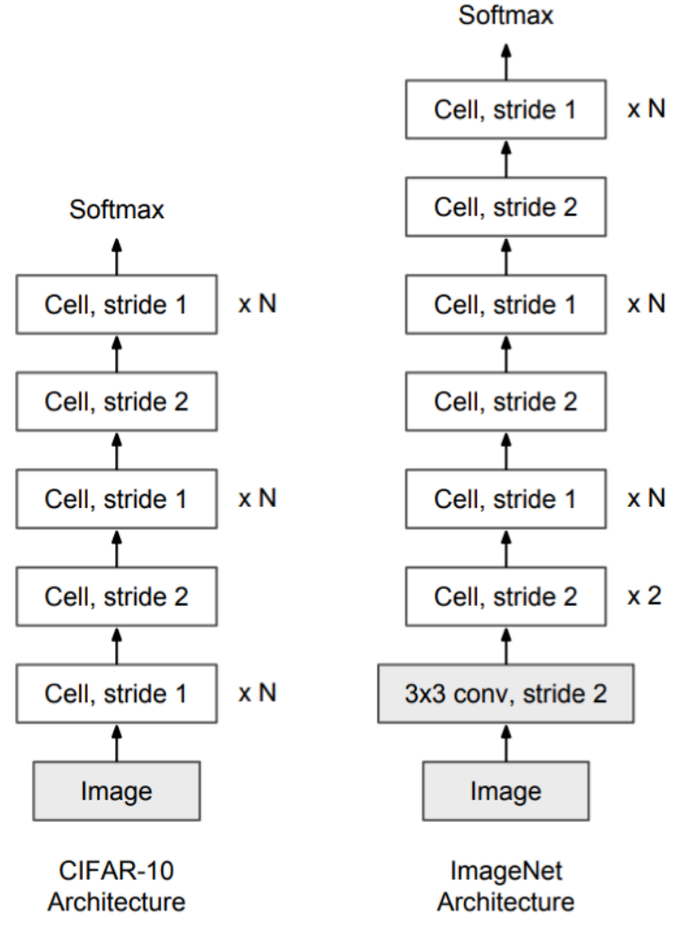


Bayesian Optimization

[1] Mendoza et al. 2016
[2] Zela et al. 2018
[3] Liu et al. 2018

- 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

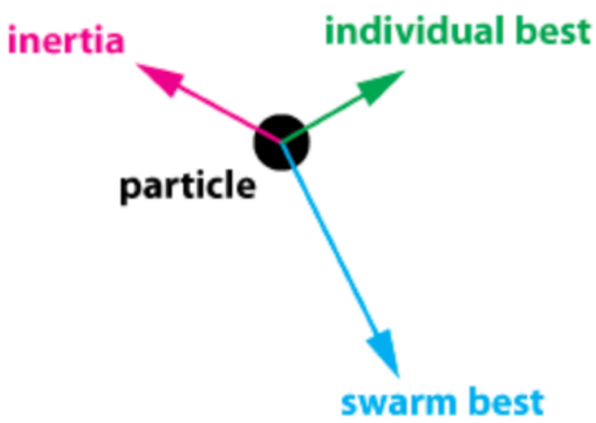


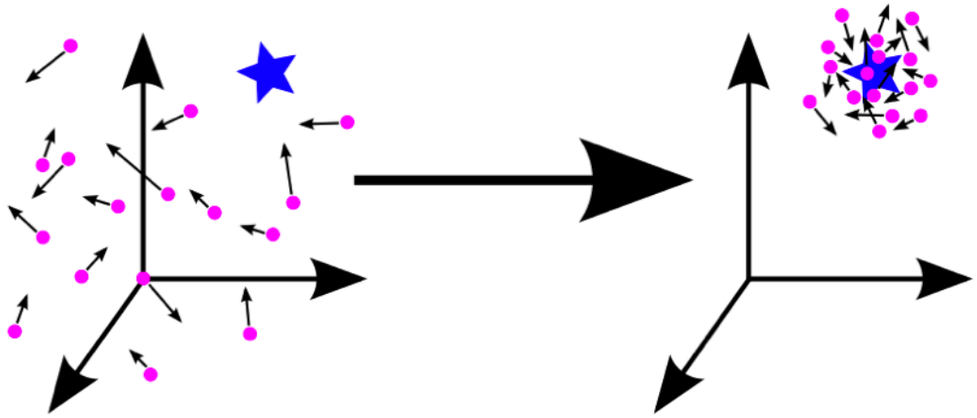


Population-based methods

- Less sample efficient, but easy to parallelize, and adapts to changes
- Genetic programming *Olson, Moore 2016, 2019*
  - Mutations: add, mutate/tune, remove HP

- Particle swarm optimization *Mantovani et al 2015*

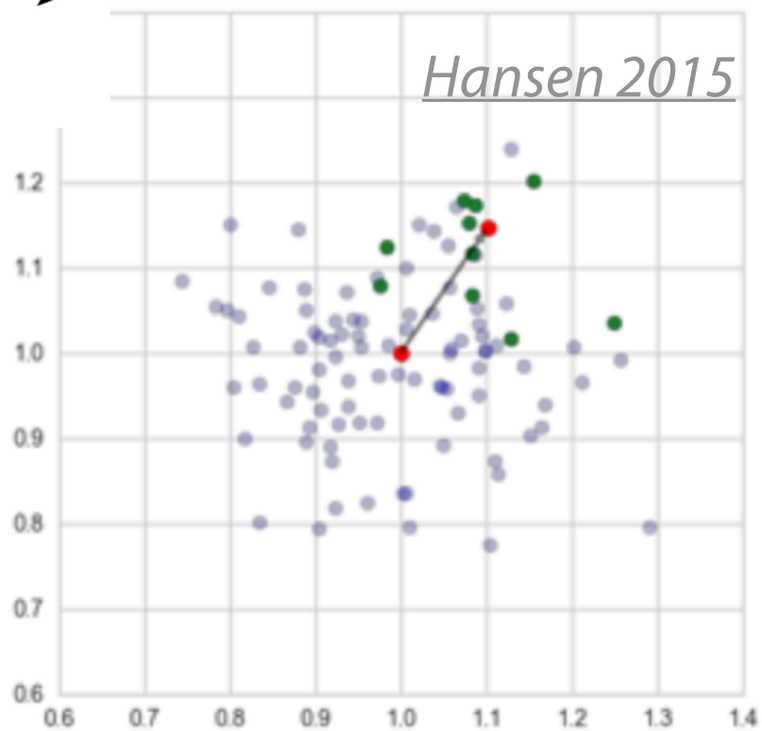




- Covariance matrix adaptation evolution (CMA-ES)
  - Purely continuous, expensive
  - Very competitive to optimize deep neural nets

[Loshilov, Hutter 2016]

Hansen 2015

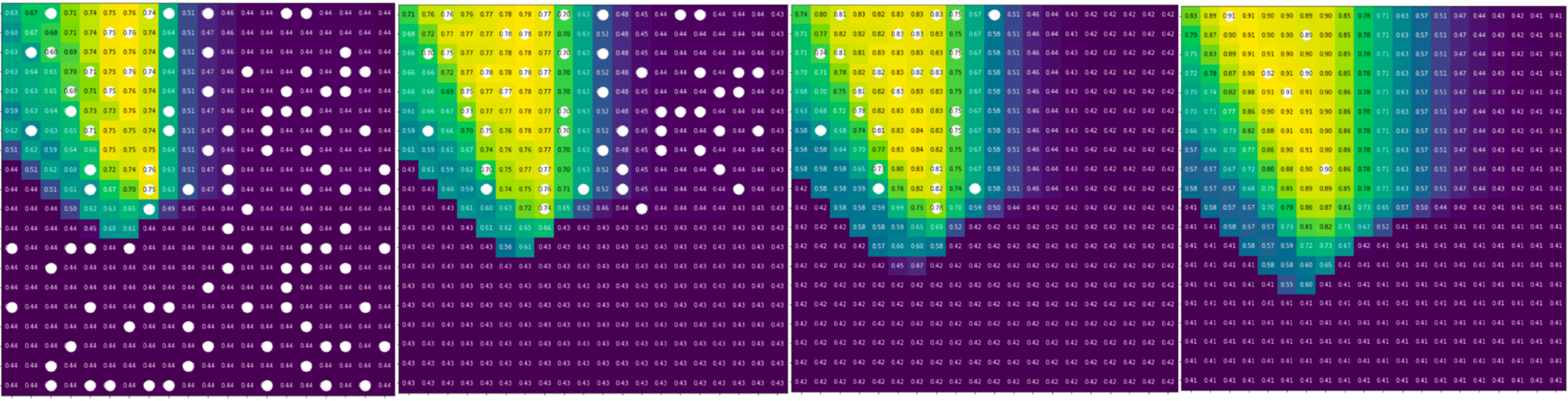


Jamieson & Talwalkar 2016

Multi-fidelity optimization

Successive halving:

- train on small subsets, infer which regions may be interesting to evaluate in more depth
- Randomly sample candidates and evaluate on a small data sample
- retrain the 50% best candidates on twice the data

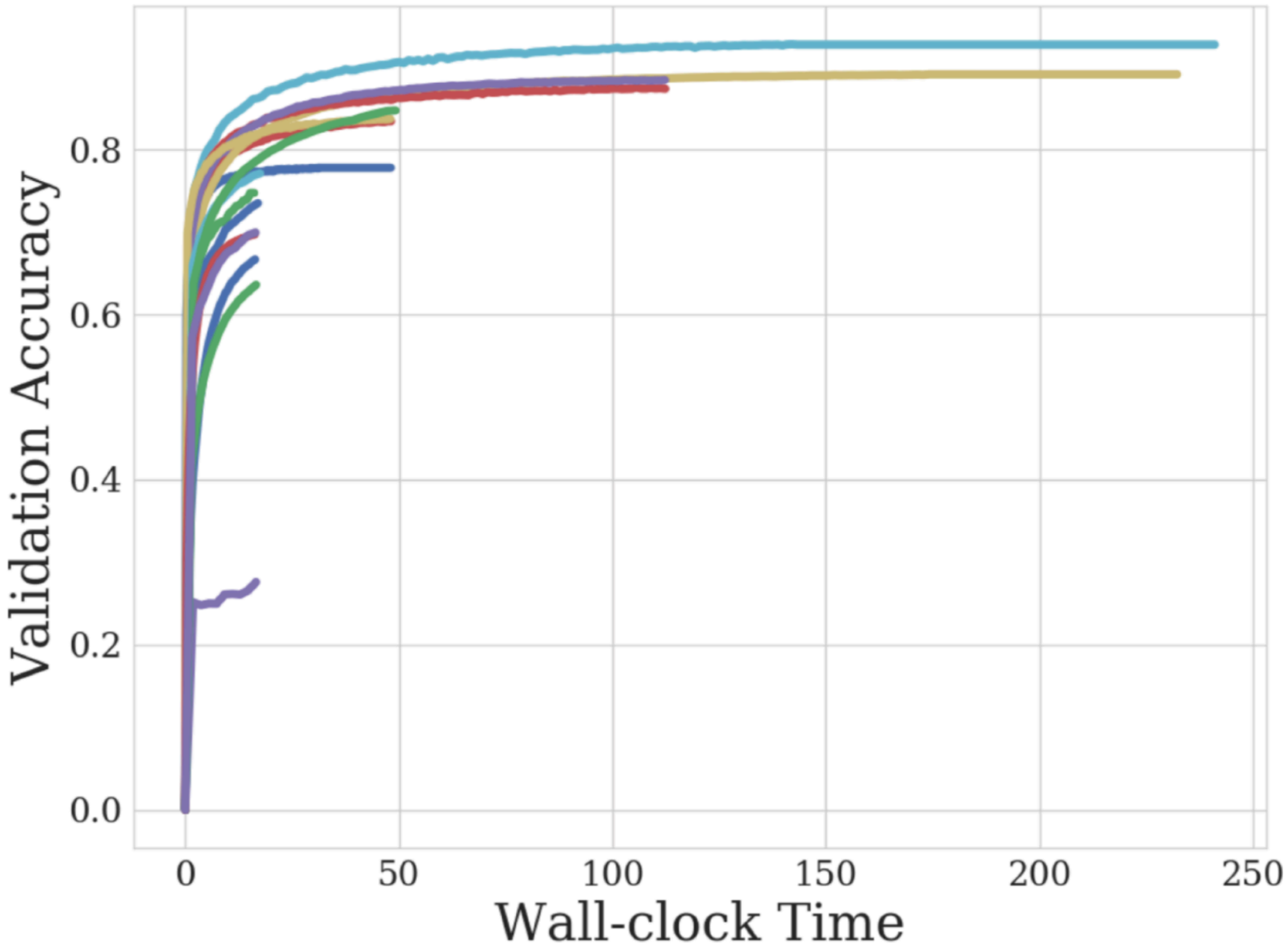


Jamieson & Talwalkar 2016

Multi-fidelity optimization

Successive halving:

- Randomly sample candidates and evaluate on a small data sample
- retrain the best half candidates on twice the data

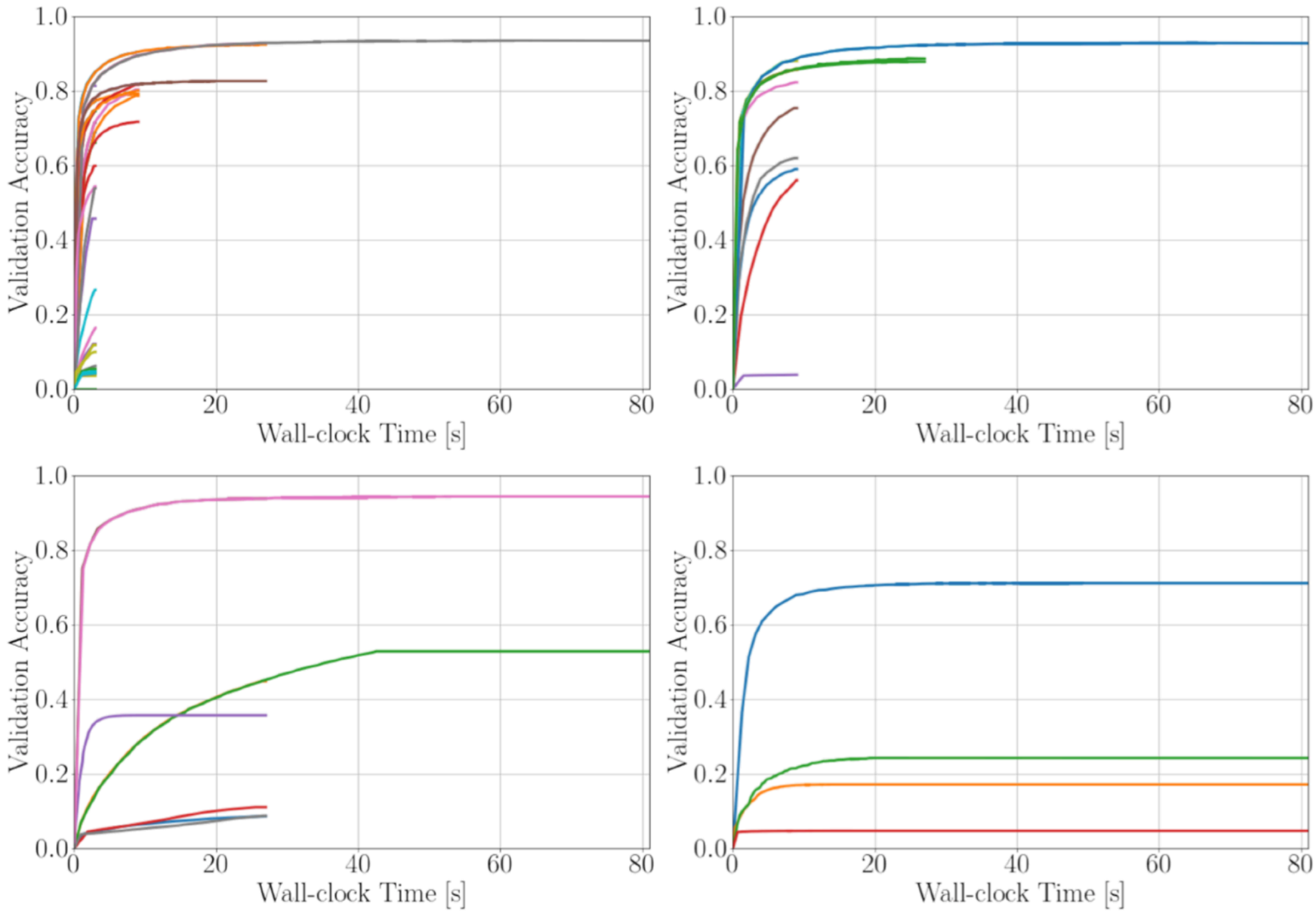


Li et al. 2017

Multi-fidelity optimization

Hyperband (HB): Repeated, decreasingly aggressive successive halving

- Minimizes (doesn't eliminate) chance that candidate was pruned to early
- Strong anytime performance, easy to implement, scalable, parallelizable

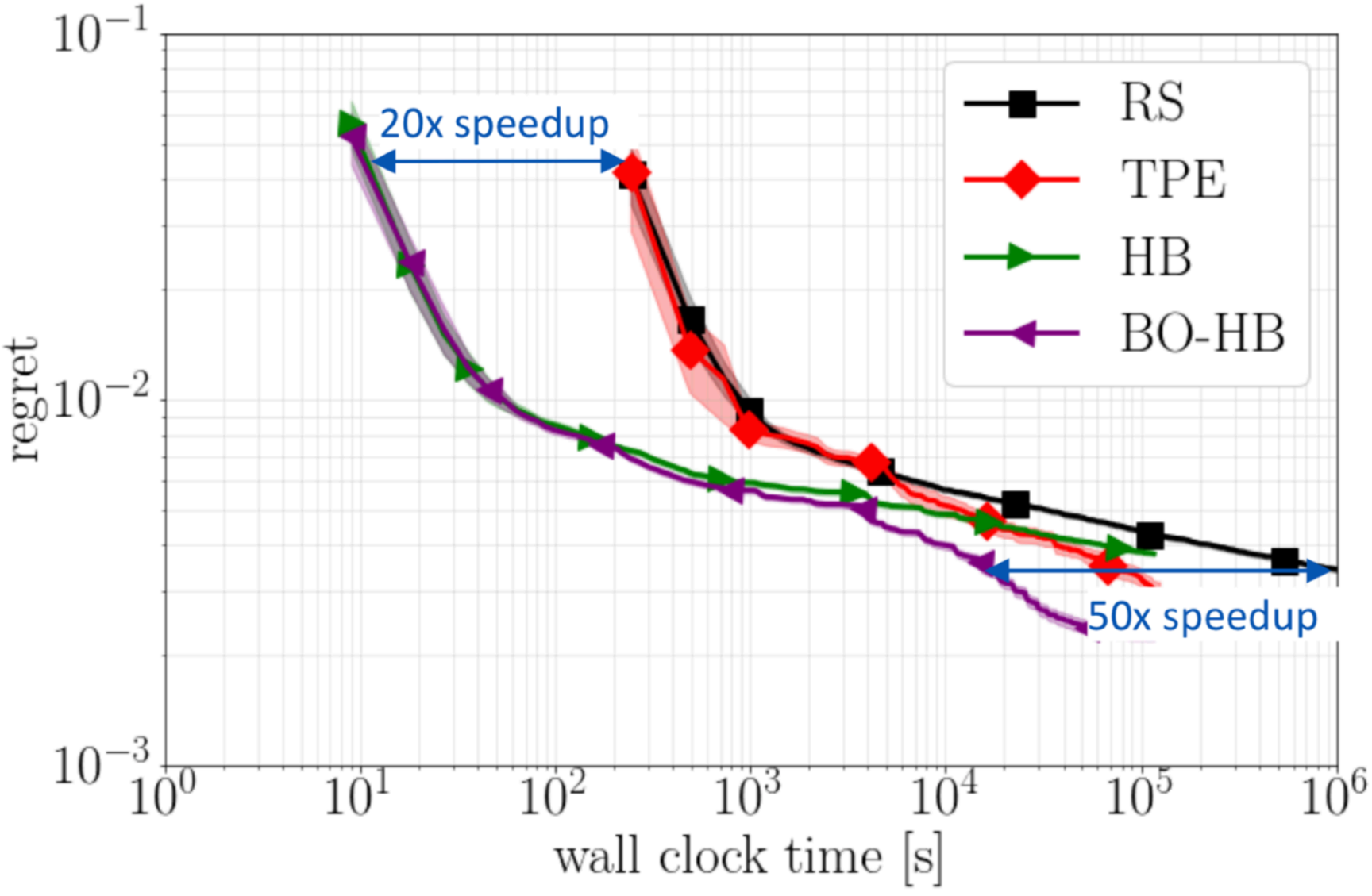


Falkner et al. 2018

Multi-fidelity optimization

Combined Bayesian Optimization and Hyperband (BO-HB)

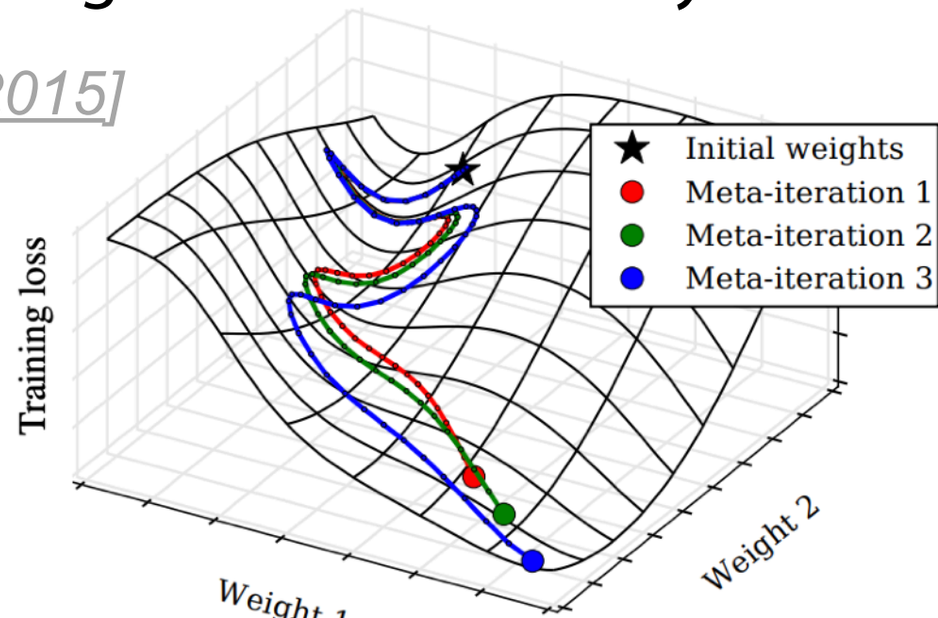
- Choose which configurations to evaluate (with TPE)
- Hyperband: allocate budgets more efficiently
- Strong anytime and final performance



Hyperparameter gradient descent

Optimize neural network hyperparameters and weights simultaneously

- Derive through the entire SGD *[MacLaurin et al 2015]*
  - Get *hypergradients* wrt. validation loss
  - Expensive! But useful if you have many hyper parameters and high parallelism



- Bilevel program *[Franceschi et al 2018]*
  - Outer obj.: optimize λ
  - Inner obj.: optimize weights given λ
    - Typically approximated

$$\begin{aligned} &\min_\lambda \ \mathcal{L}_{val}\left(w^*(\lambda), \lambda\right) \\ s.t. \quad &w^*(\lambda) = \operatorname{argmin}_w \mathcal{L}_{train}\left(w, \lambda\right) \end{aligned}$$

- Interleave optimization steps *[Luketina et al 2016]*
  - Alternate SGD steps for ω and λ

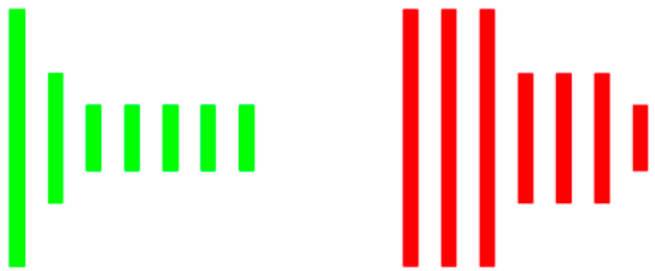
Hyperparameter gradient step w.r.t. $\nabla_\lambda \mathcal{L}_{val}$

Parameter gradient step w.r.t. $\nabla_w \mathcal{L}_{train}$

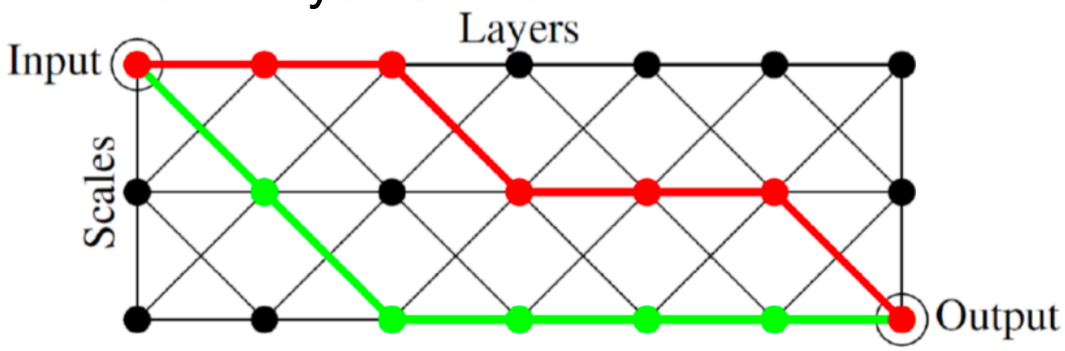
Weight Sharing

[1] Saxena & Verbeek, 2016
[2] Bender et al. 2018
[3] Pham et al. 2018
[4] Brock et al. 2017

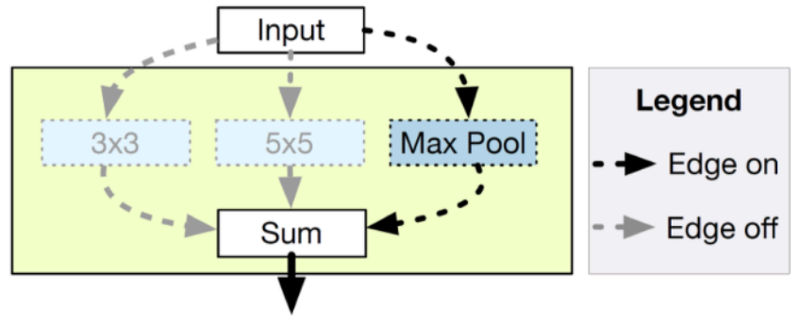
- One-shot models (fixed architecture, or *neural fabric*) [1]
  - Search space: ConvNet = path though *fabric* with shared weights
  - Train ensemble of all of them



For 7-layer CNNs:



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

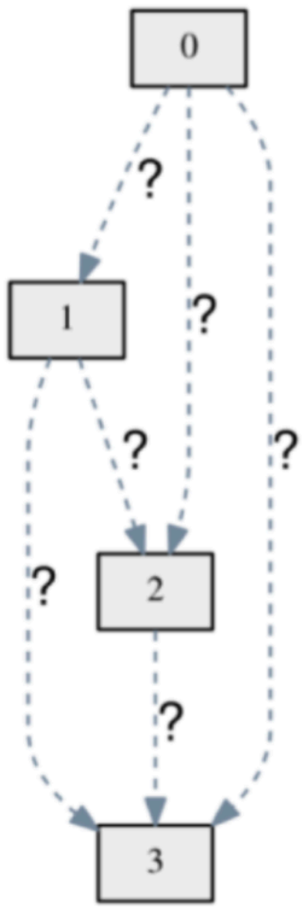


- *ENAS* [3]
  - use RL to sample paths from one-shot model, train weights
  - other paths inherit these weights
- *SMASH* [4]
  - Shared hypernetwork that predicts weights given architecture

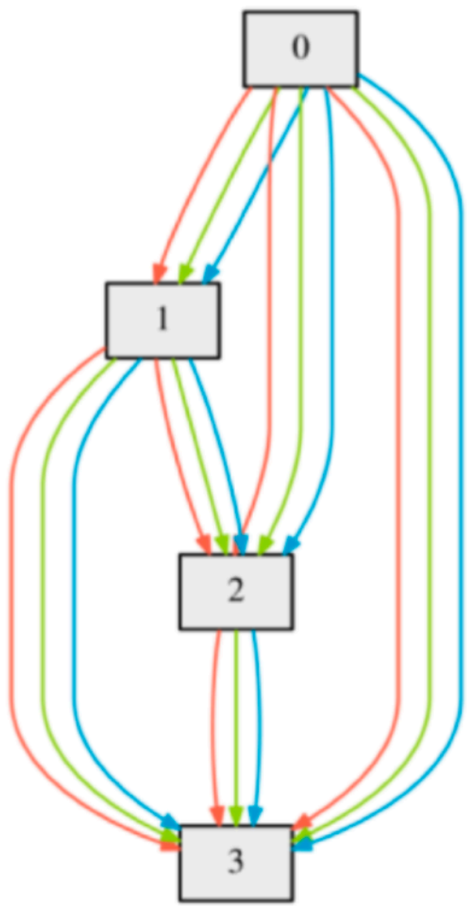
Liu et al. 2018

DARTS: Differentiable NAS

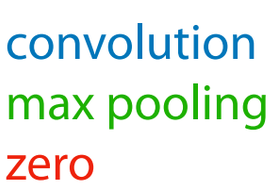
- Fixed (one-shot) structure, learn which operators to use
- Give all operators a weight α_i
- Optimize α_i and model weights ω_j using bilevel optimization
  - approximate $\omega_j^*(\alpha_i)$ by adapting ω_j after every training step

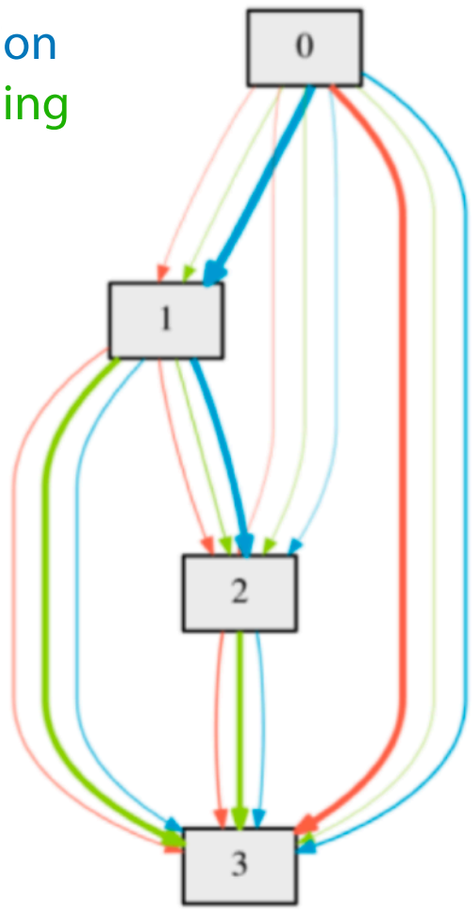


One-shot model

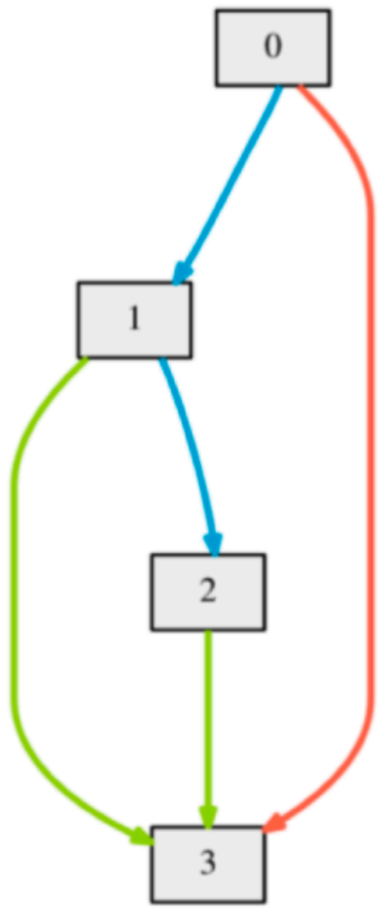


operator weights α_i





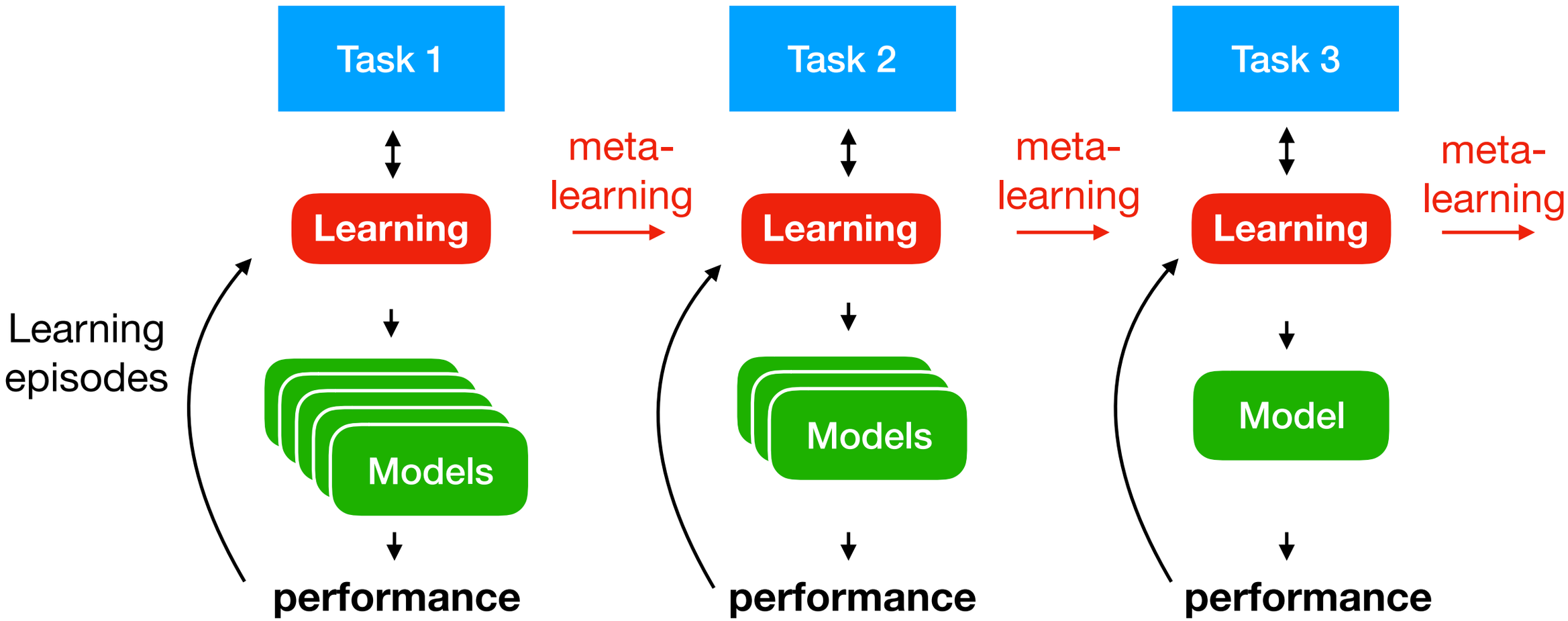
interleaved optimization of α_i and ω_j with SGD



argmax α_i

Learning is a never-ending process

Humans learn *across* tasks
Why? Requires less trial-and-error, less data



Learning is a never-ending process

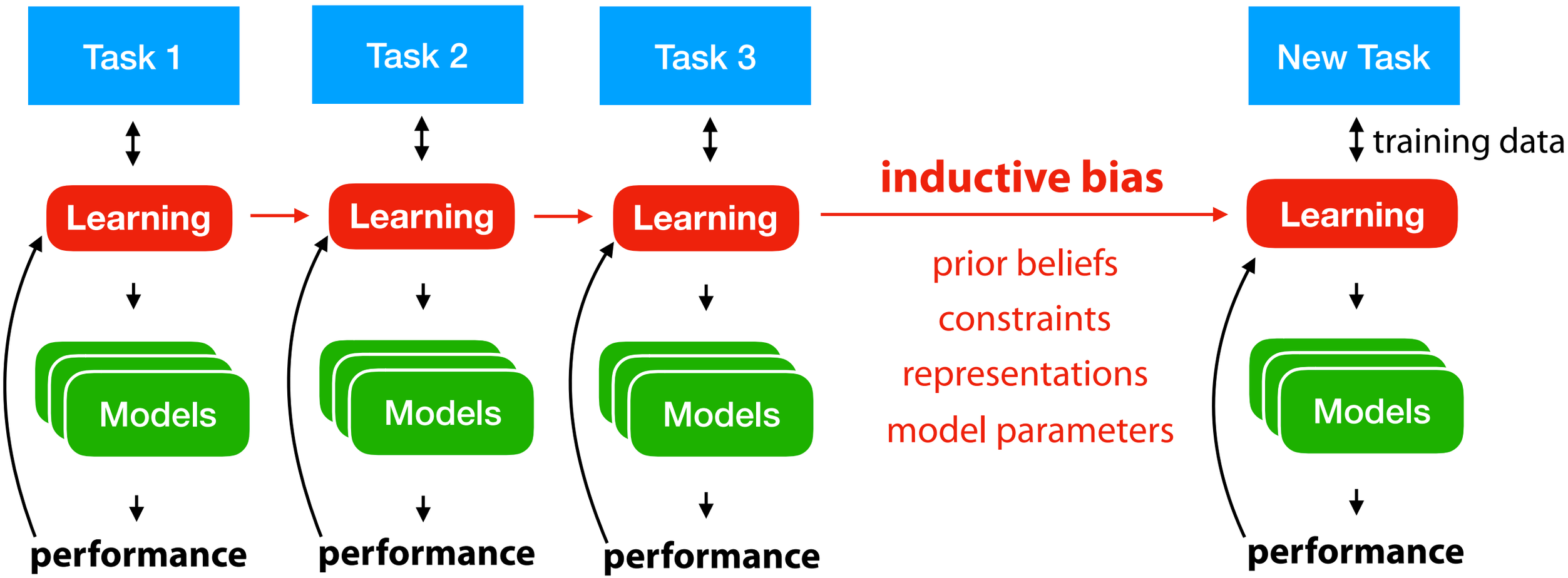
Learning humans also seek/create related tasks

E.g. find many similar puzzles, solve them in different ways,…

Learning to learn

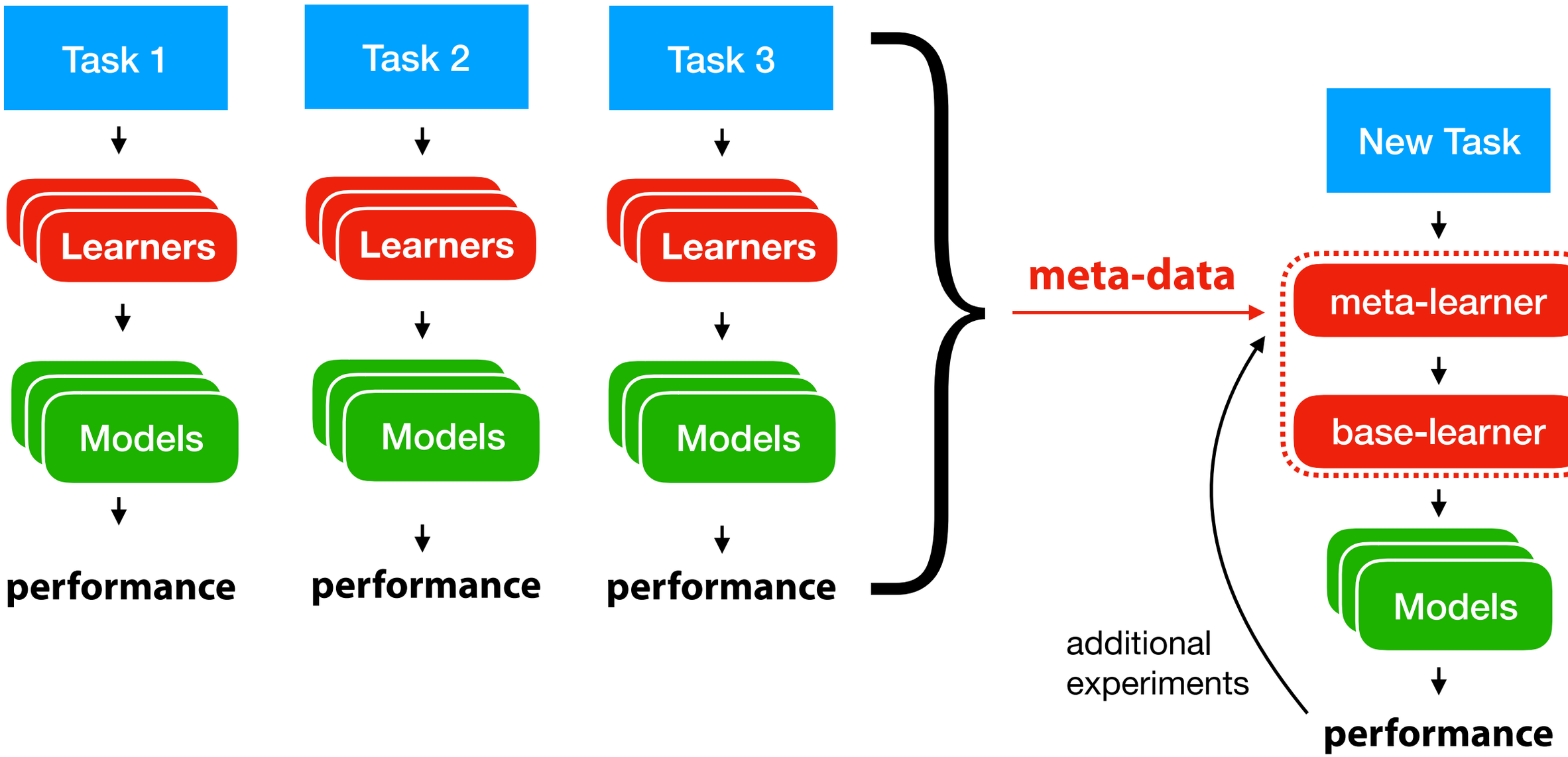
If prior tasks are *similar*, we can ***transfer*** prior knowledge to new tasks

Inductive bias: assumptions added to the training data to learn effectively



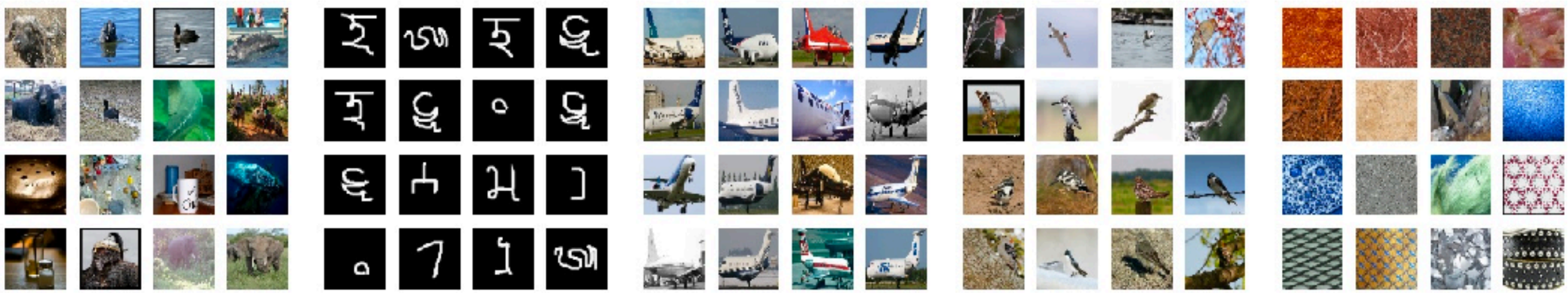
Meta-learning

Meta-learner *learns* a (base-)learning algorithm, based on *meta-data*

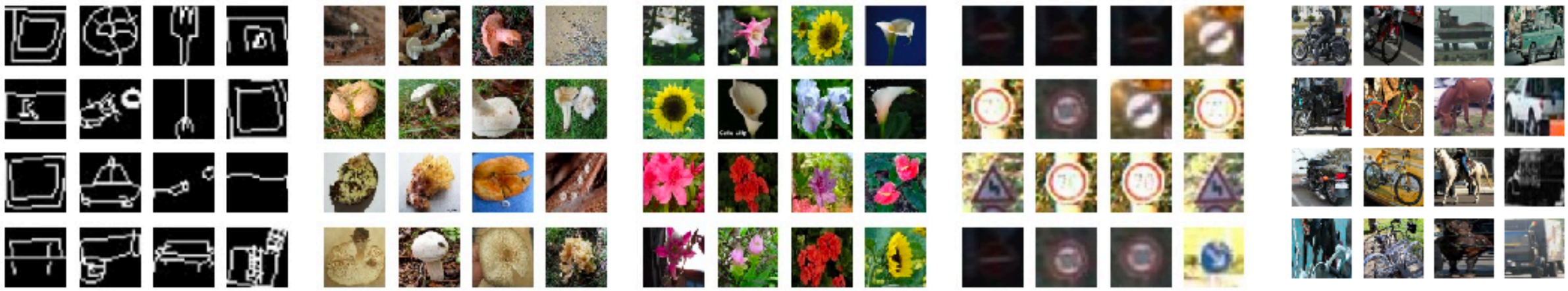


Triantafillou et al. 2019

Example: meta-dataset



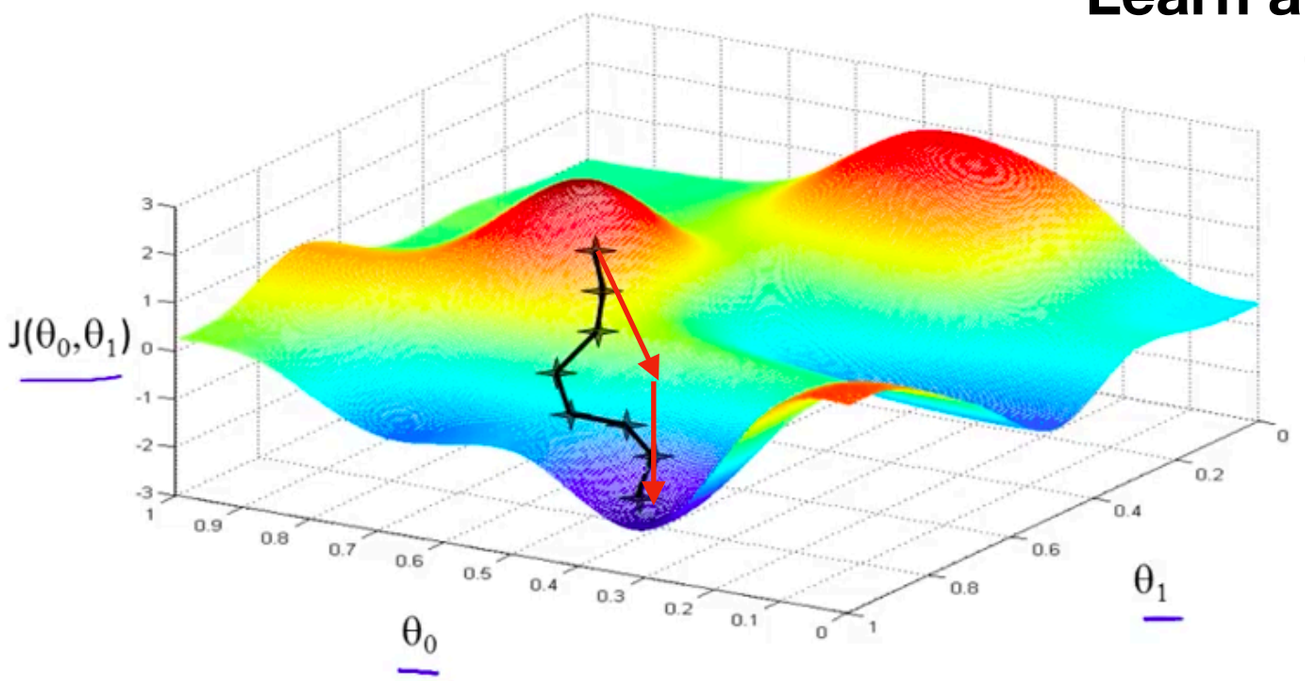
(a) ImageNet (b) Omniglot (c) Aircraft (d) Birds (e) DTD

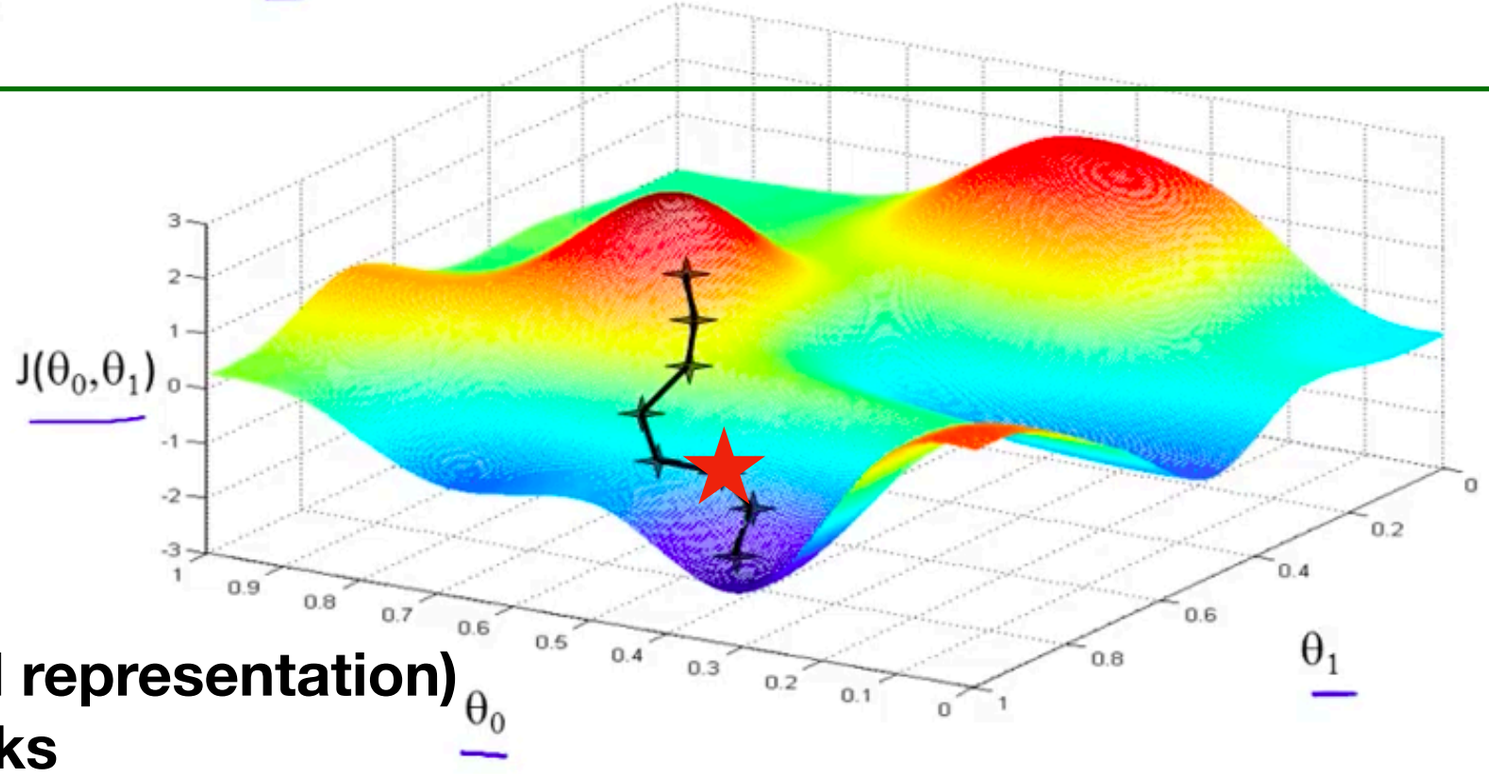


(f) Quick Draw (g) Fungi (h) VGG Flower (i) Traffic Signs (j) MSCOCO

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] Bengio et al. 1995

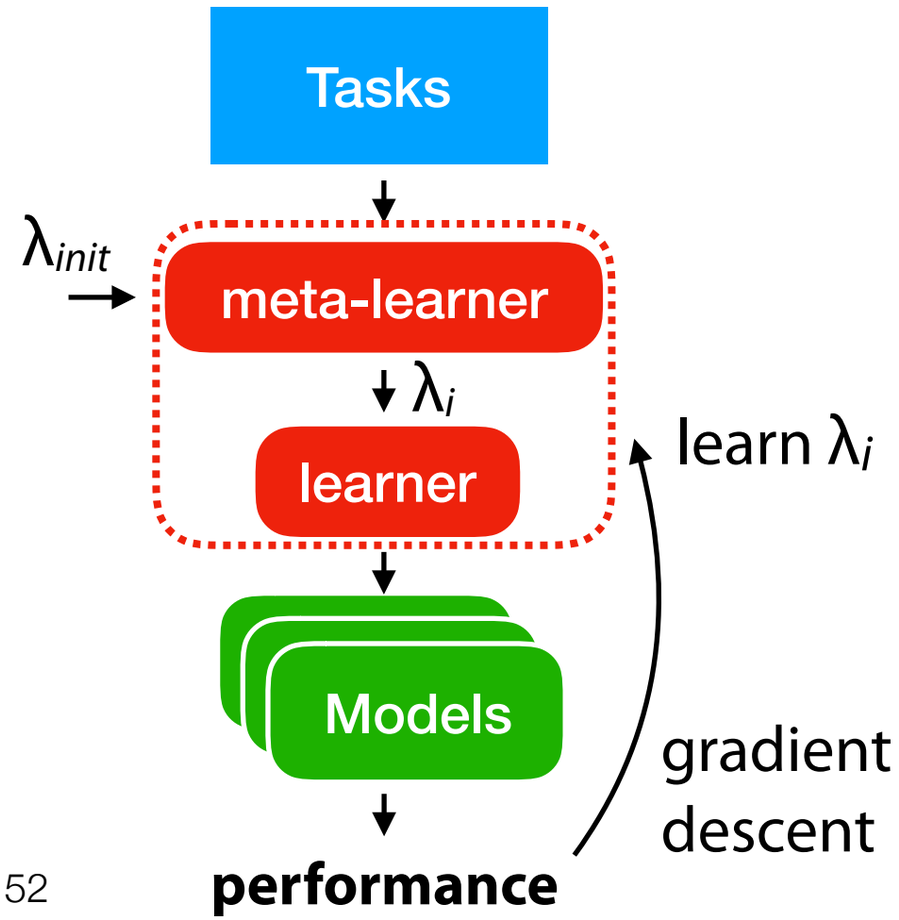
[2] Runarsson and Jonsson 2000

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.

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

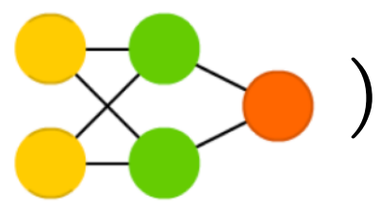
presynaptic activity

learning rate

reinforcing signal

Runarsson and Jonsson

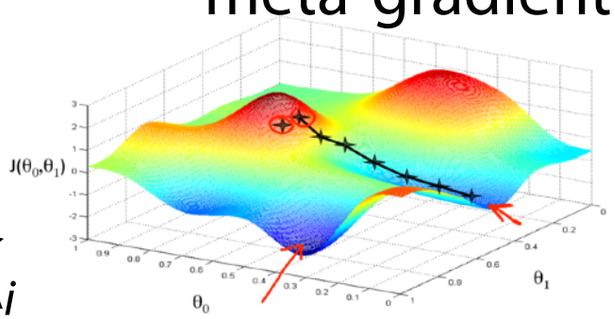
$$\Delta \theta_i = \eta \, (\quad)$$



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

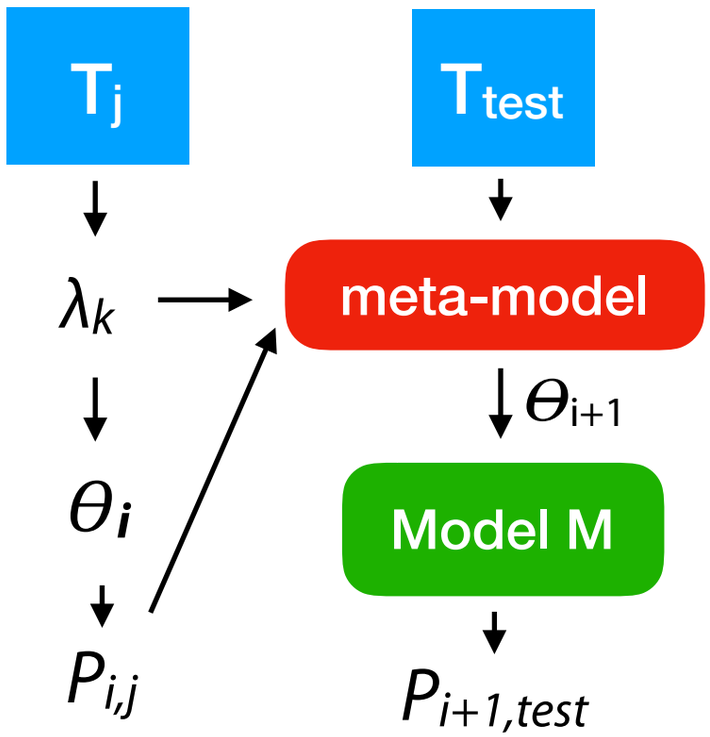
Learning to learn gradient descent by gradient descent

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

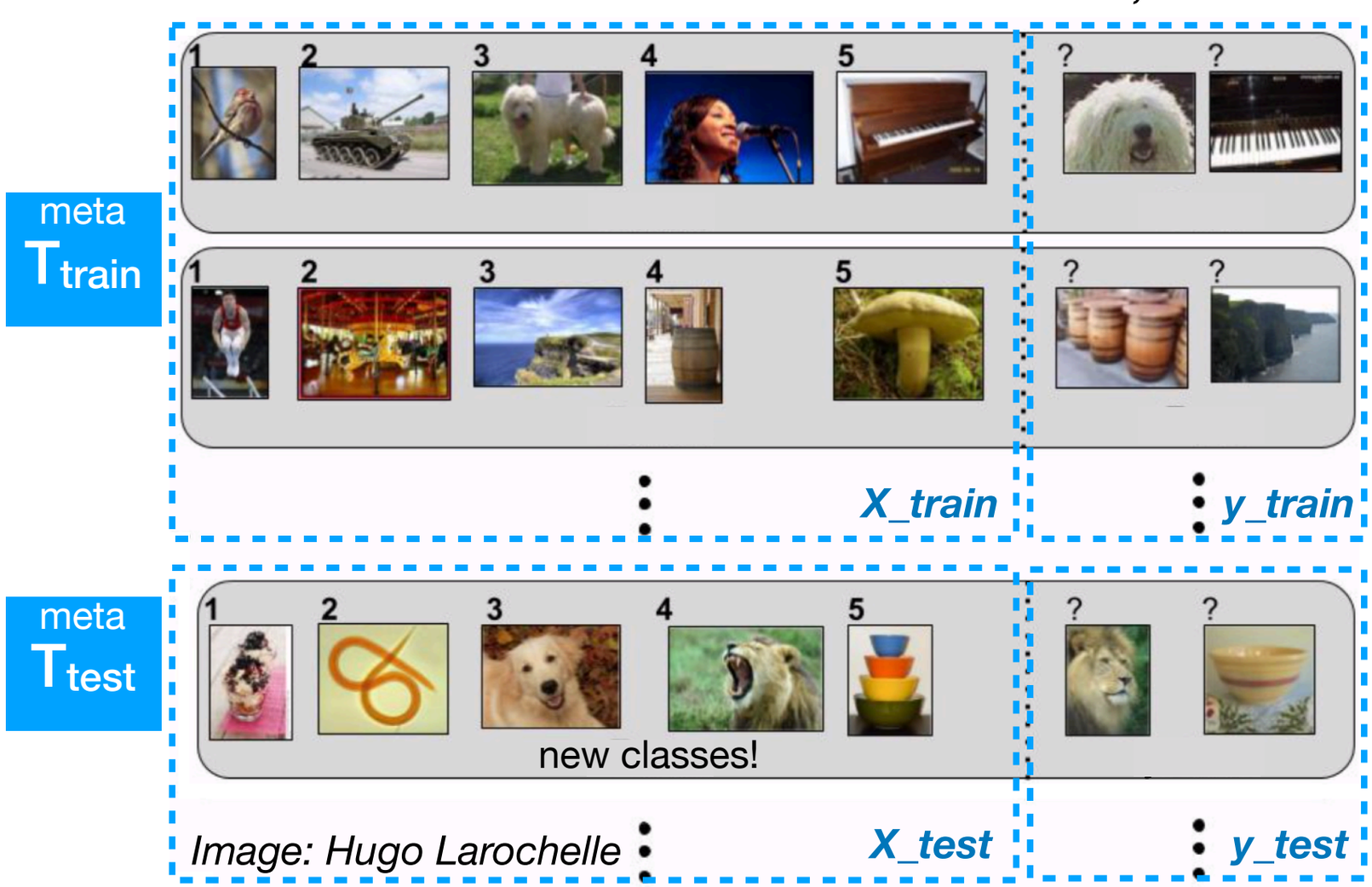
Application: Few-shot learning

- 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

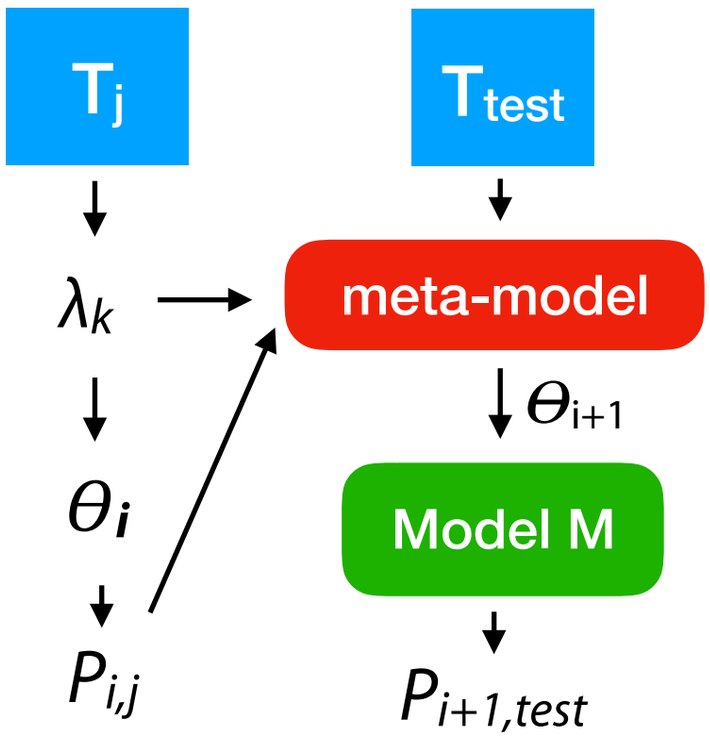
$$Cost(\theta_i) = \frac{1}{|T_{test}|} \sum_{t \in T_{test}} loss(\theta_i, t)$$



1-shot, 5-class:



Few-shot learning: approaches



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

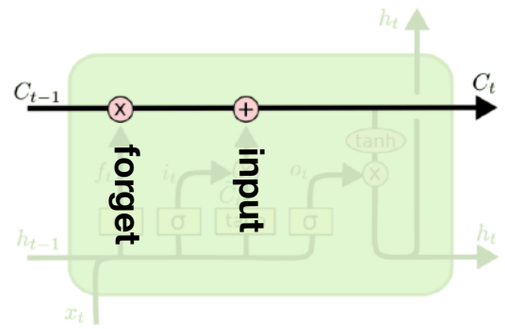
- Existing algorithm as meta-learner:
  - LSTM + gradient descent — *Ravi and Larochelle 2017*
  - Learn θ_{init} + gradient descent — *Finn et al. 2017*
  - kNN-like: Memory + similarity — *Vinyals et al. 2016*
  - Learn embedding + classifier — *Snell et al. 2017*
  - …
- Black-box meta-learner
  -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

Ravi and Larochelle 2017

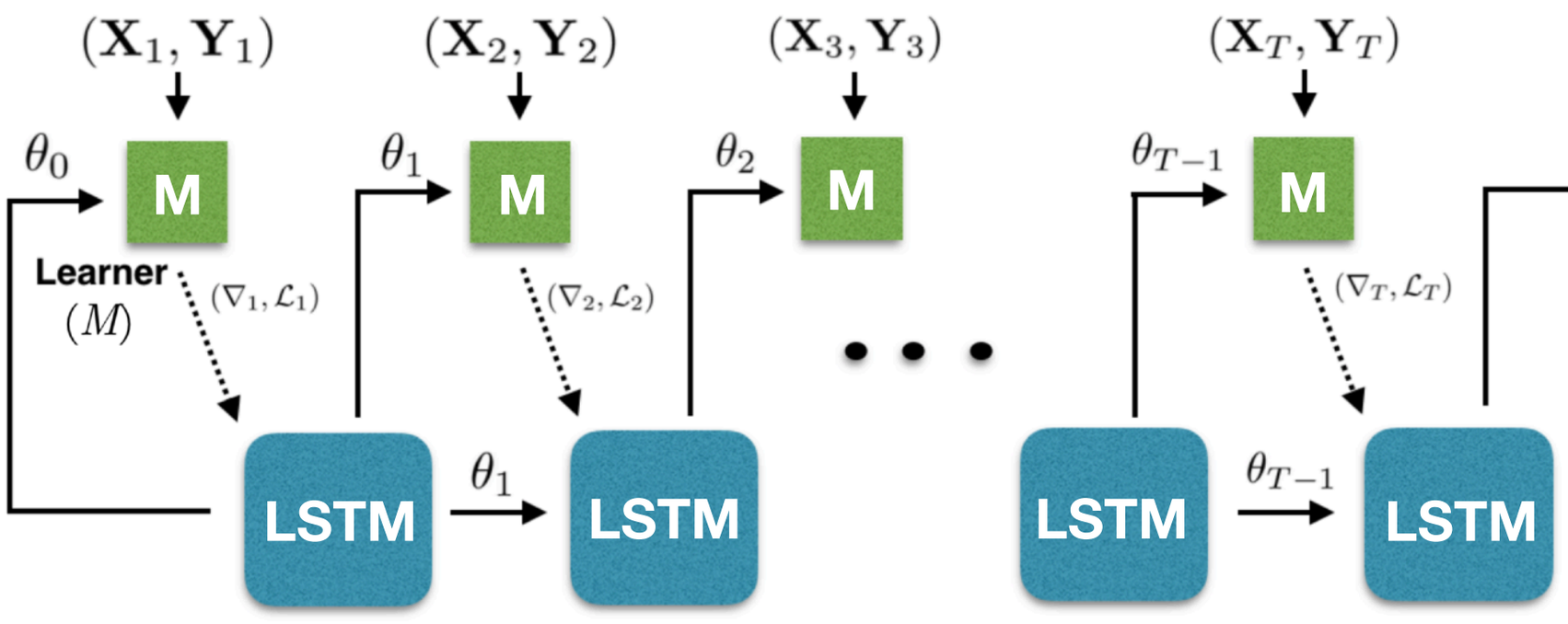
LSTM meta-learner + gradient descent

- 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

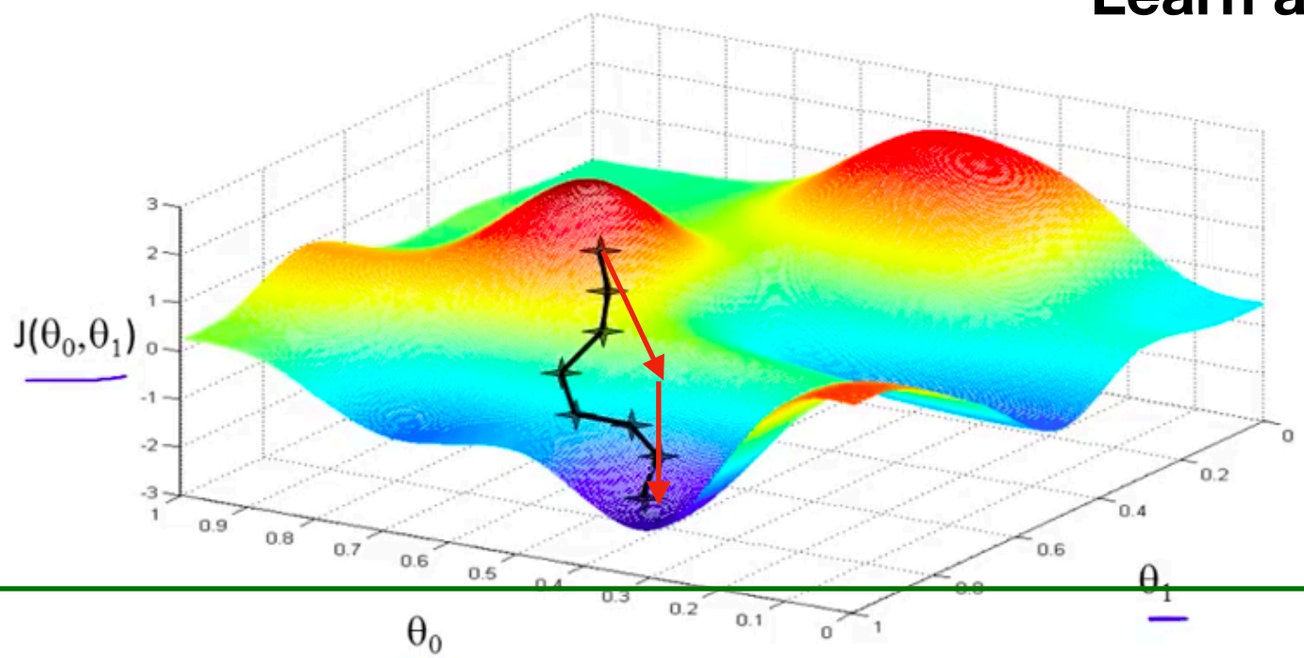


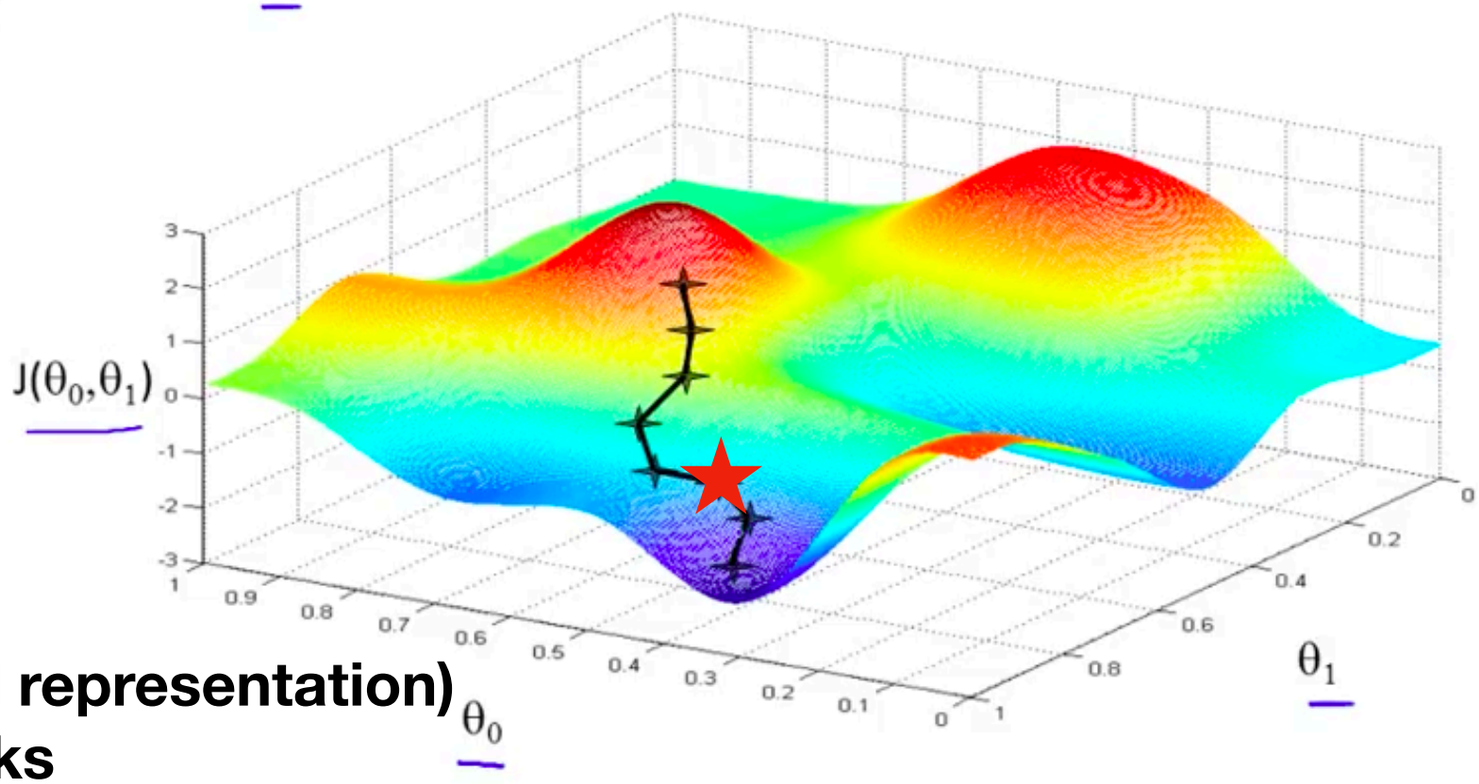
$$Cost(\theta_T) = \frac{1}{|T_{test}|} \sum_{t \in T_{test}} loss(\theta_T, t)$$

Train | Test

Learning to learn

Learn a better gradient update rule for a group of tasks



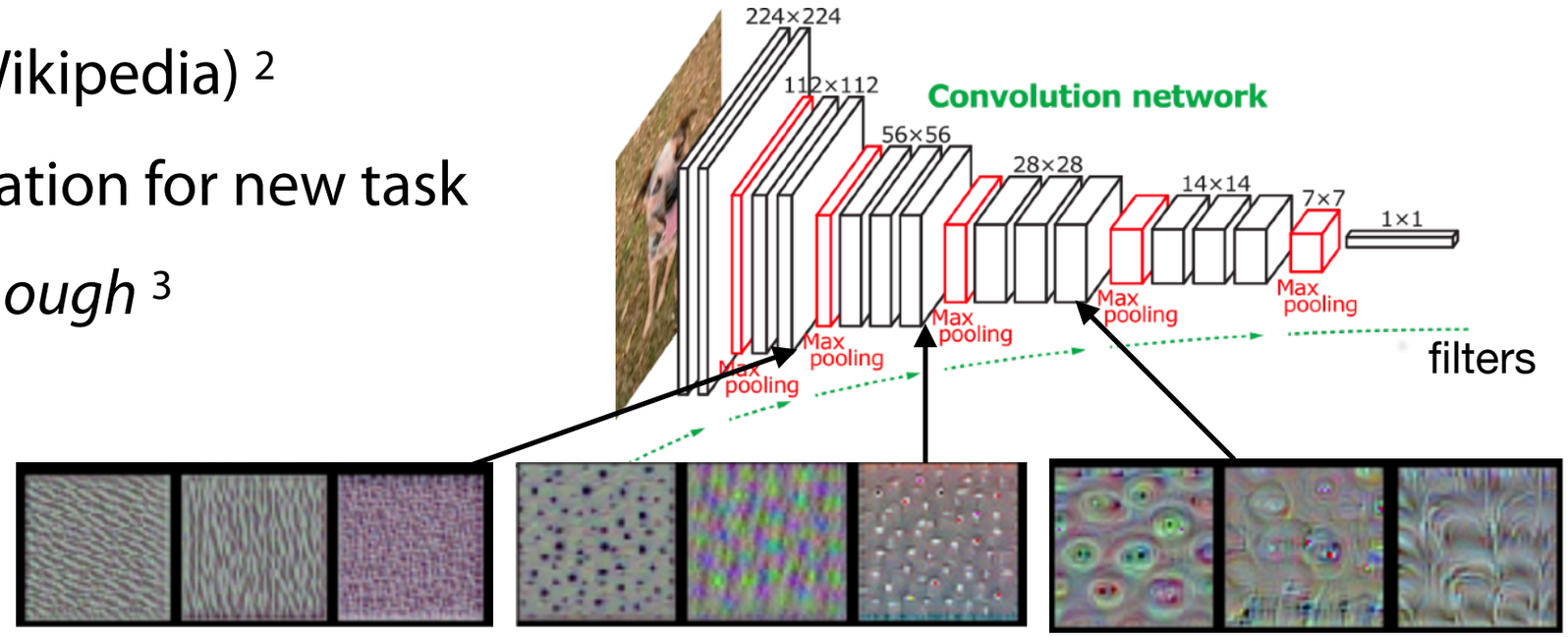


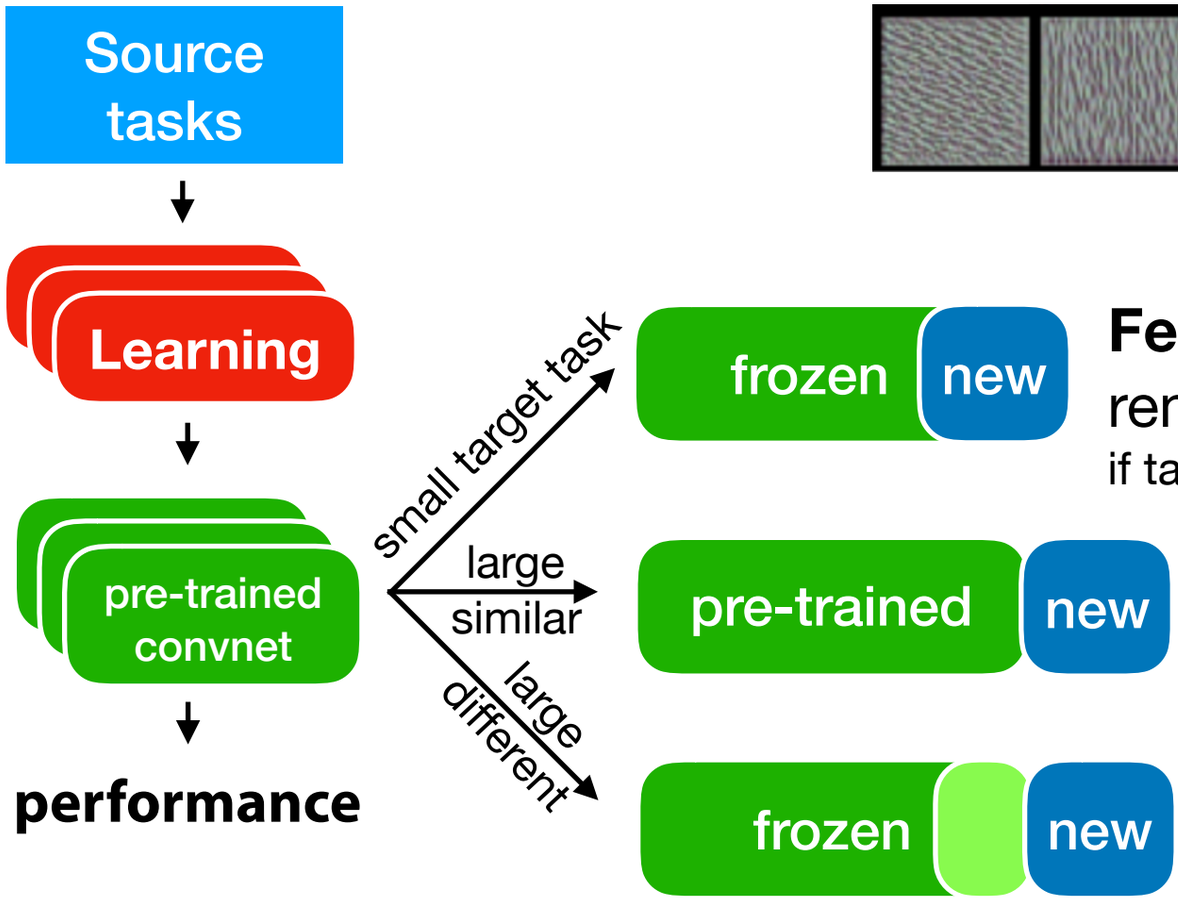
Learn a better initialization (and representation) for a group of tasks

Transfer learning

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

- 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

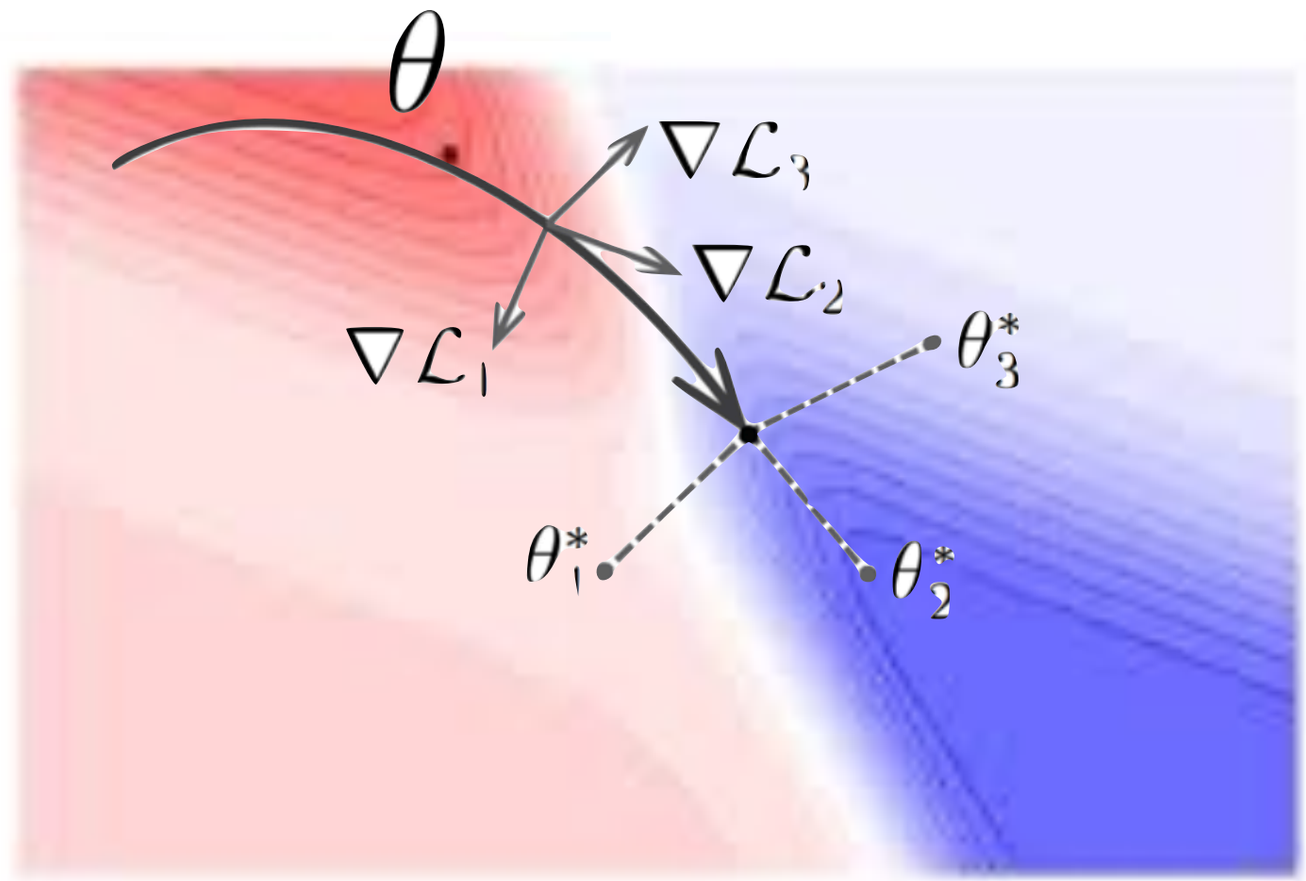
[1] Finn et al. 2017

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



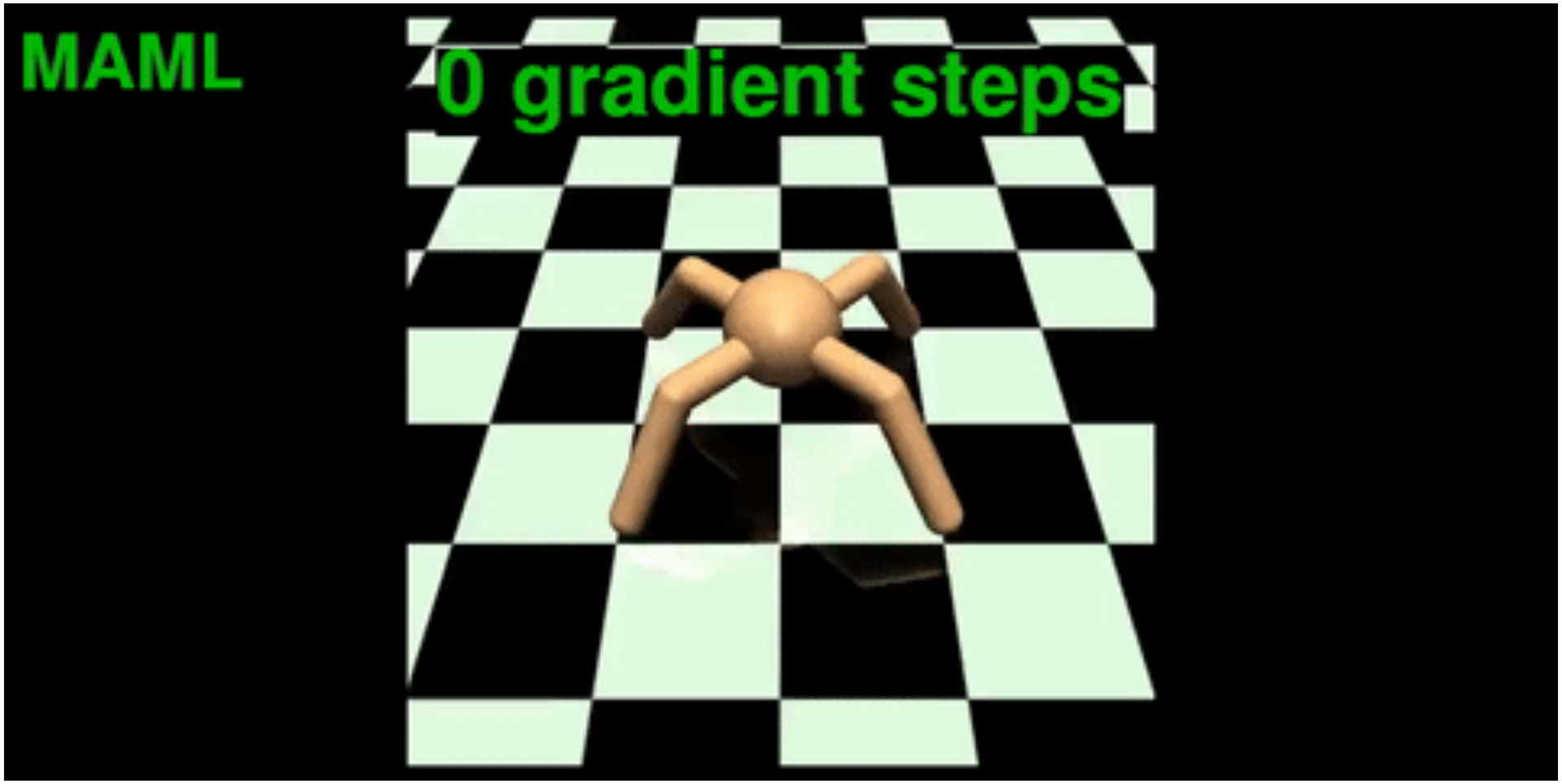
[1] Finn et al. 2018
[2] Nichol et al. 2018

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
  - …
- Lots of current research
  - What does it actually learn?
  - Can it work on out-of-distribution, multi-modal task distributions,…?

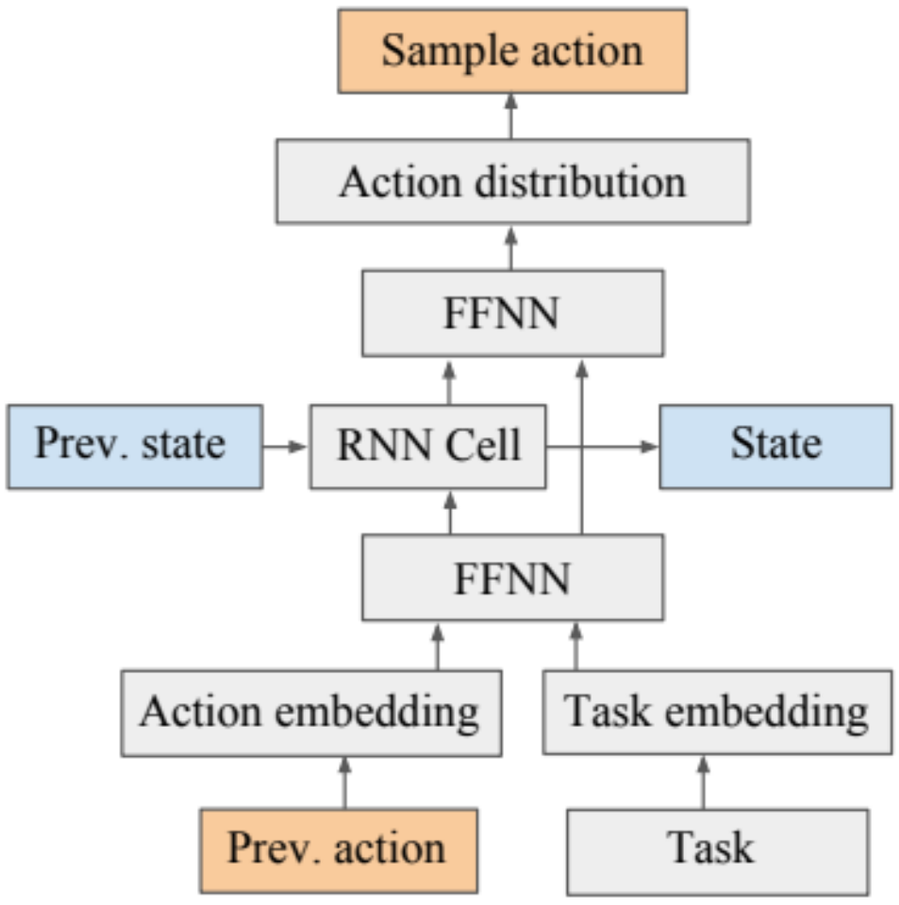
Model-agnostic meta-learning

- 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

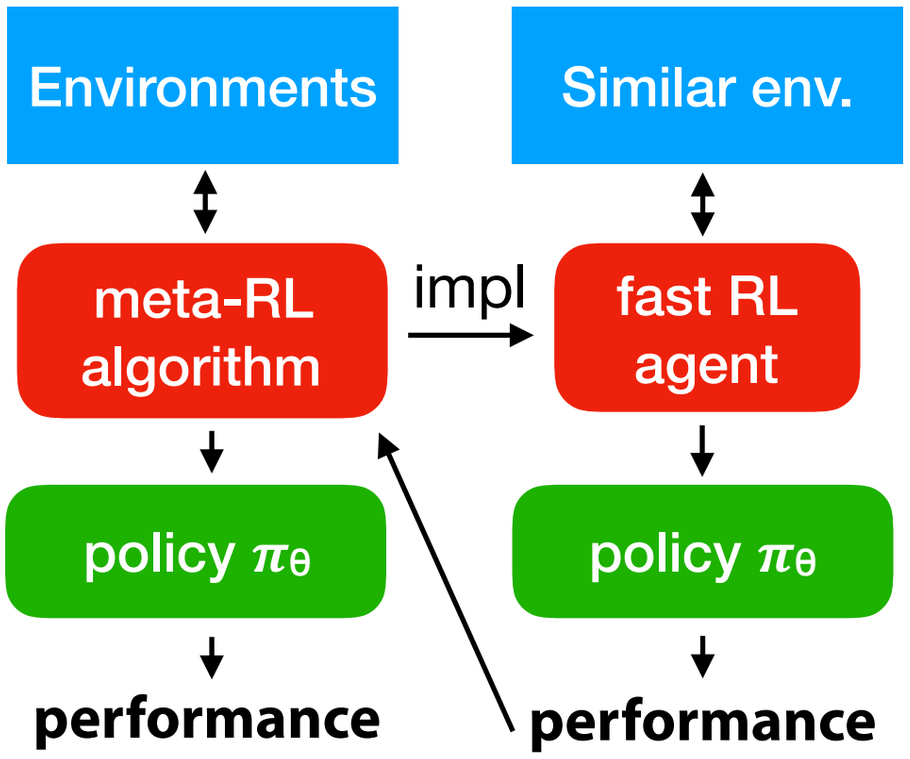


- Another idea: warm-start DARTS with task-specific one-shot model

Learning to reinforcement learn

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

- 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

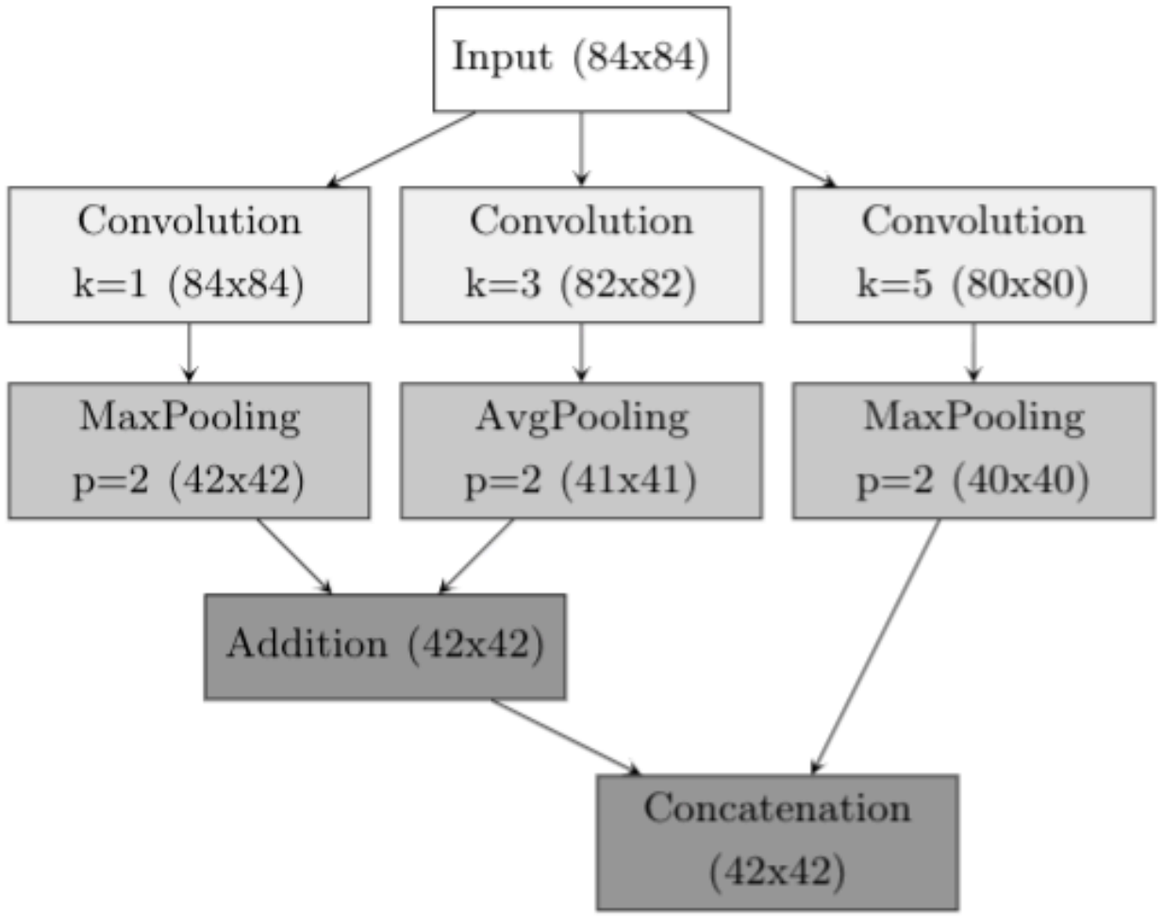
Gomez & Vanschoren, NeurIPS 2019

Meta-Reinforcement Learning for NAS

- Train an agent how to build a neural net, across tasks
- Should transfer but also adapt to new tasks

[0, 0, 0, 0, 0]
[0, 0, 0, 0, 0]
[1, 1, 1, 0, 0]
[2, 2, 2, 1, 0]
[3, 1, 3, 0, 0]
[4, 3, 2, 3, 0]
[5, 1, 5, 0, 0]
[6, 2, 2, 5, 0]
[7, 5, 0, 2, 4]
[8, 7, 0, 0, 0]

Actions: add certain layers in certain locations

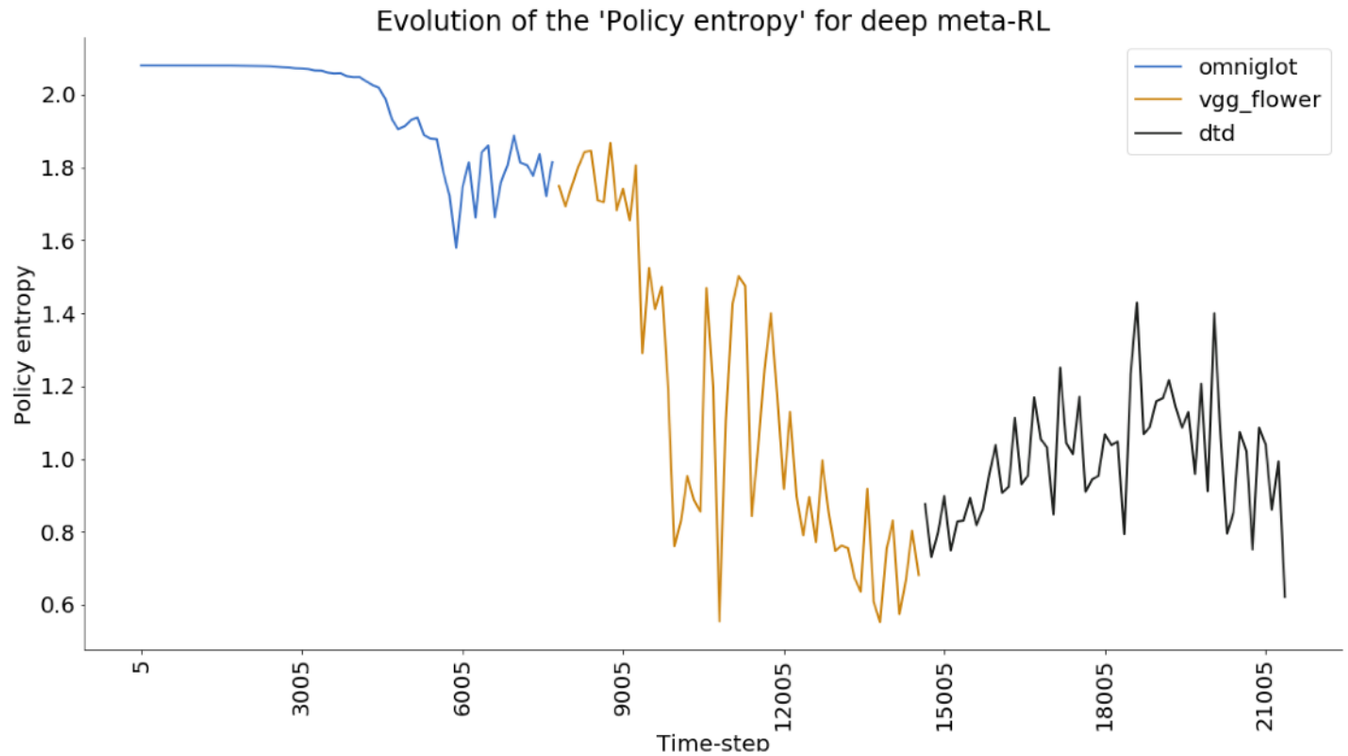


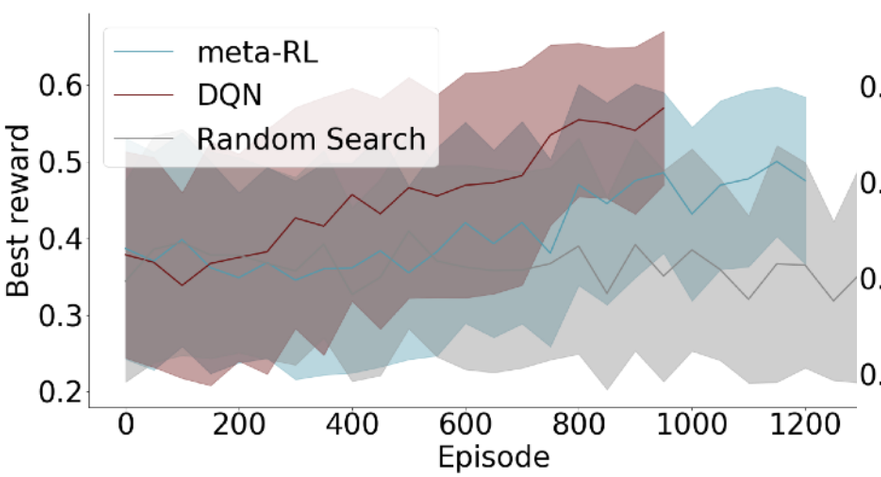
Gomez & Vanschoren, NeurIPS 2019

Meta-Reinforcement Learning for NAS

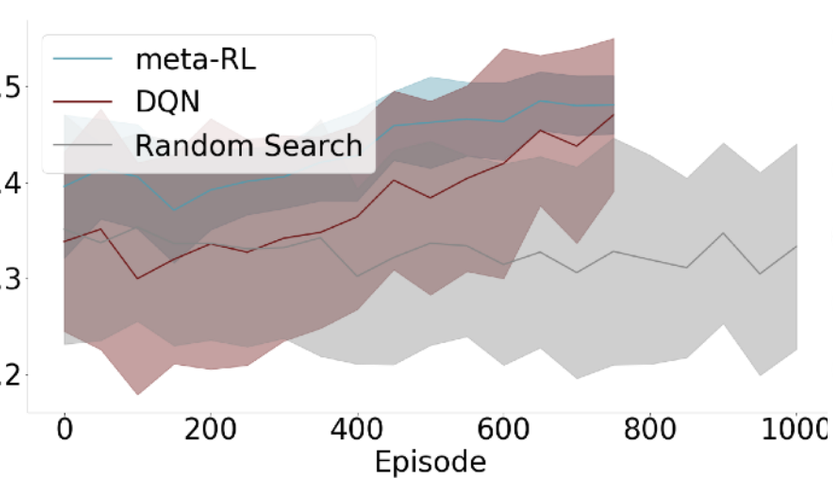
Results on increasingly difficult tasks:

- omniglot
- vgg_flower
- dtd

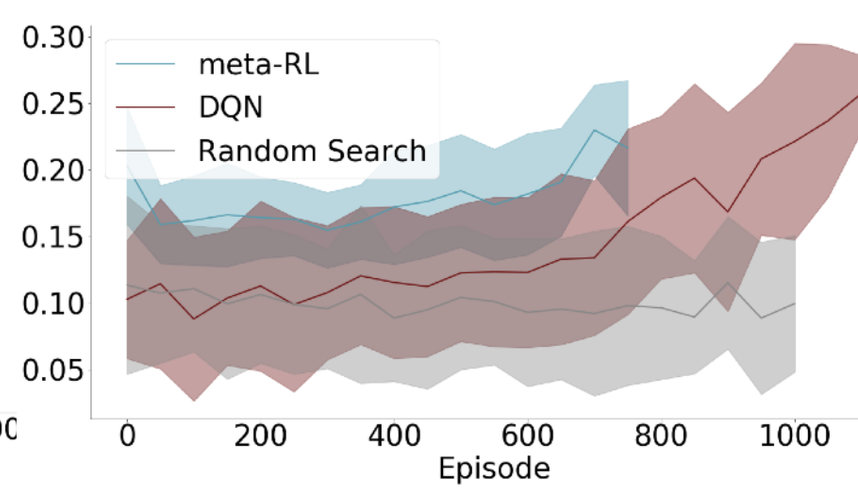




omniglot



vgg_flower



dtd

Meta-learning for less similar tasks

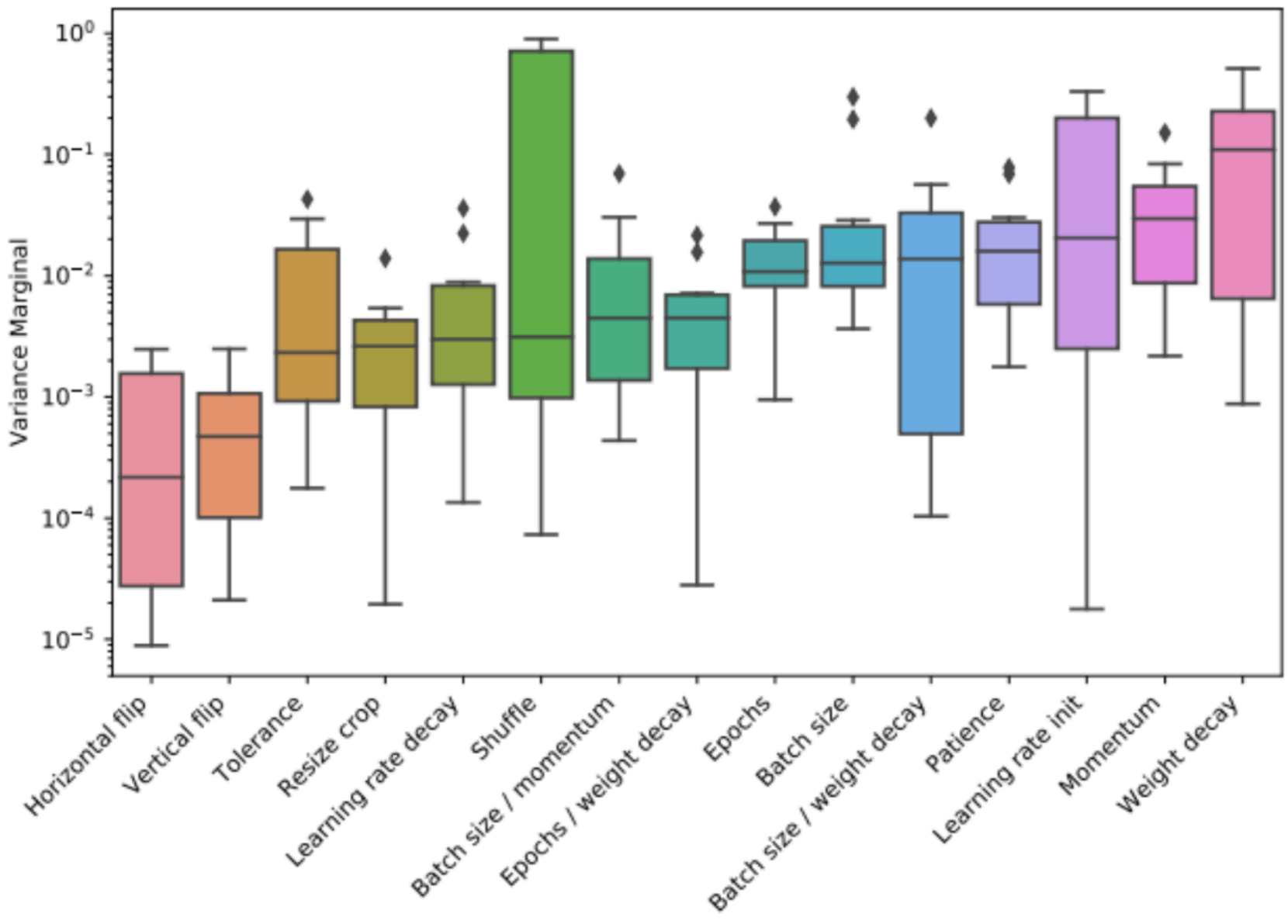
Meta-learning can also speed up the architecture and hyperparameter search, in combination with the optimization techniques we just discussed

- Learn which hyperparameters are really important
- Learn which hyperparameter values should be tried first
- Learn which architectures will most likely work
- Learn which feature representations to use
- Learn which embeddings, pre-trained nets to use
- …

[1] van Rijn & Hutter 2018

Meta-learning for Hyperparameter optimization

- **Functional ANOVA** [1]
  Select hyperparameters that cause variance in the evaluations.

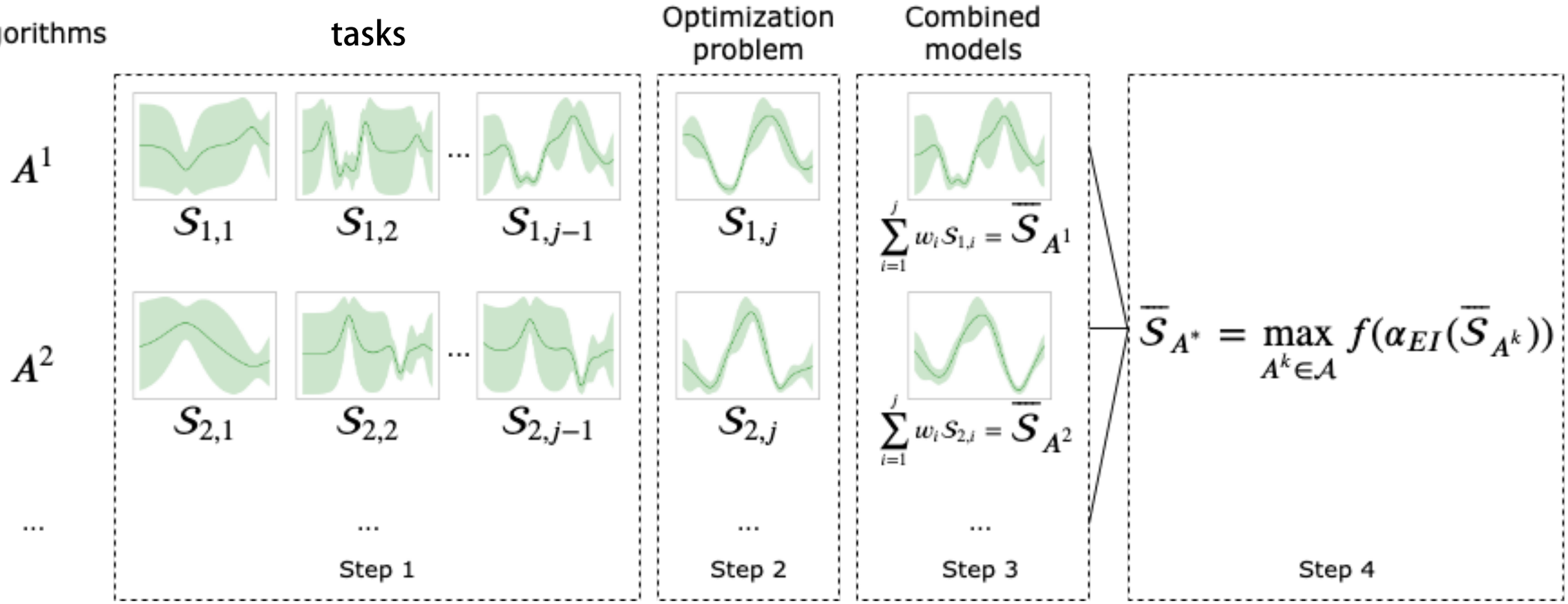


ResNets for image classification

Feurer et al., ICML 2018
Manolache & Vanschoren, NeurIPS 2019

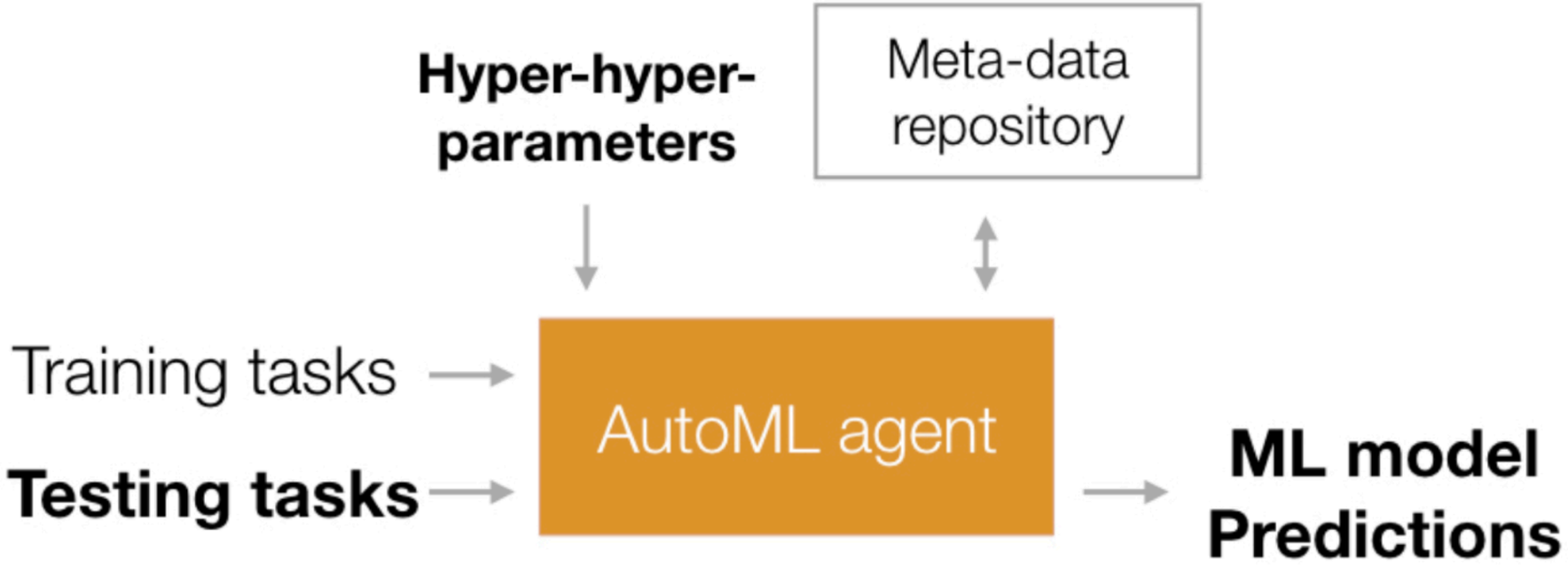
Meta-Learning for Bayesian Optimization

- **Surrogate model transfer**
  - Store the surrogate models for previous tasks
  - Learn a weighted function over them on a new task
  - Much faster optimization (not yet tested for deep learning)

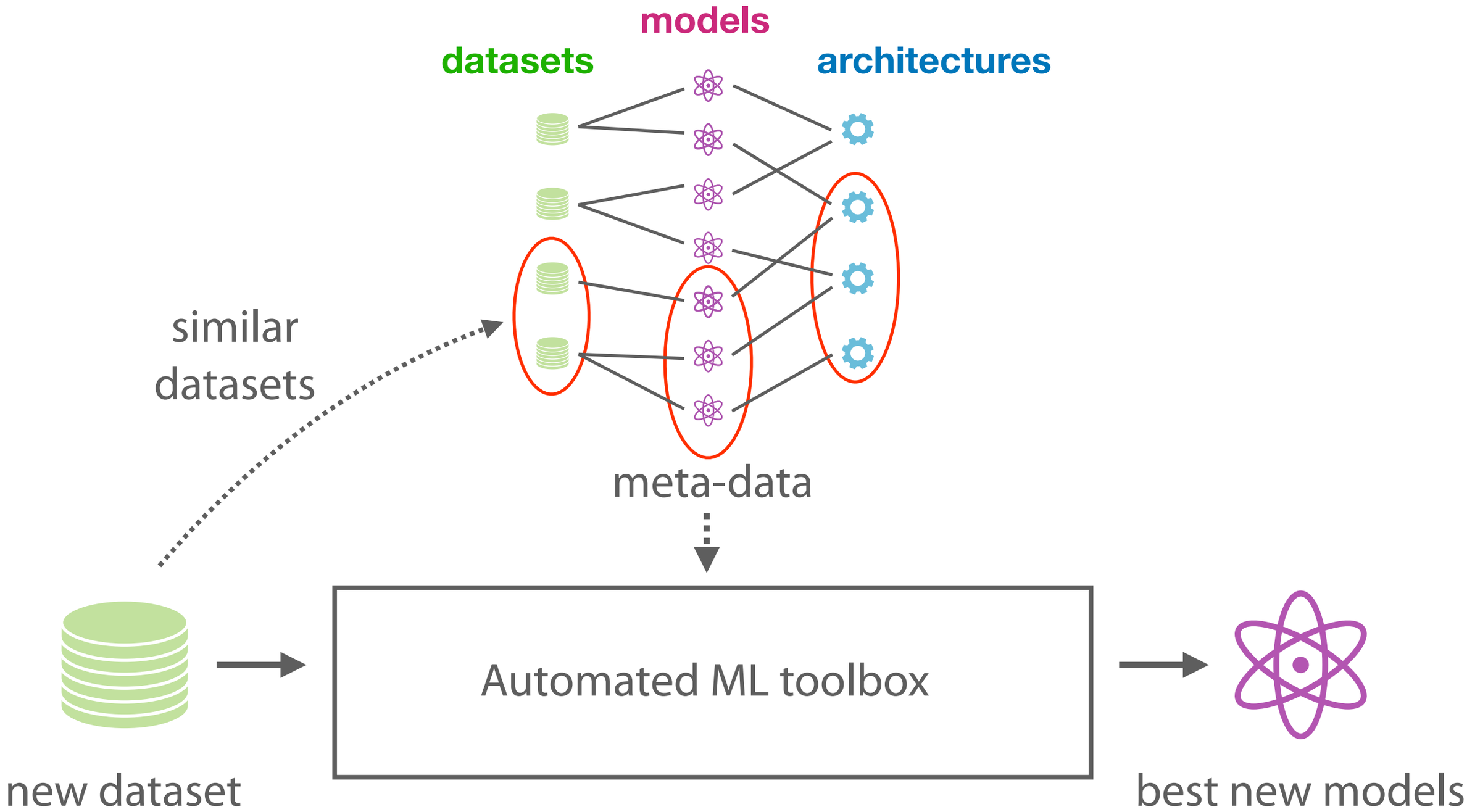


Meta-learning in practice

- We need a meta-data repository of relevant prior machine learning experiments
  - e.g. OpenML.org (needs more deep learning experiments)
- Ideally, a *shared* memory that all AutoML tools can access



Meta-learning with OpenML



AutoML *open source* tools

	Architect. search	Operators	Hyperpar. search	Improvements	Metalearnin
Auto-WEKA	Param. pipeline	WEKA	Bayesian Opt. (RF)		
auto-sklearn	Param. pipeline	sklearn	Bayesian Opt. (RF)	Ensemble	warm-start
mlr-mbo	Param. pipeline	mlr	Bayesian Opt.	multi-obj.	
BO-HB	Param. pipeline	sklearn	Tree of Parzen Estim.	Ensemble, HB	
hyperopt-sklearn	Param. pipeline	sklearn	Tree of Parzen Estim.		
skopt	Param. pipeline	sklearn	Bayesian Opt. (GP)		
TPOT	Evolving pipelines	sklearn	Population-based		
GAMA	Evolving pipelines	sklearn	Population-based	Ensemble, ASHA	
H2O AutoML	Param. pipeline	H2O	Random search	Stacking	
OBOE	Single algorithms	sklearn	Low rank approx.	Ensembling	runtime pred
Auto-Keras	Param. NAS	keras	Bayesian Opt.	Net Morphisms	
Auto-pyTorch	Param. pipeline	pyTorch	BO-HB		
TensorFlow 2	/	keras	RS or HB		
Talos	/	keras	RS variants		

Many other tools for hyperparameter optimization alone

Thank you!

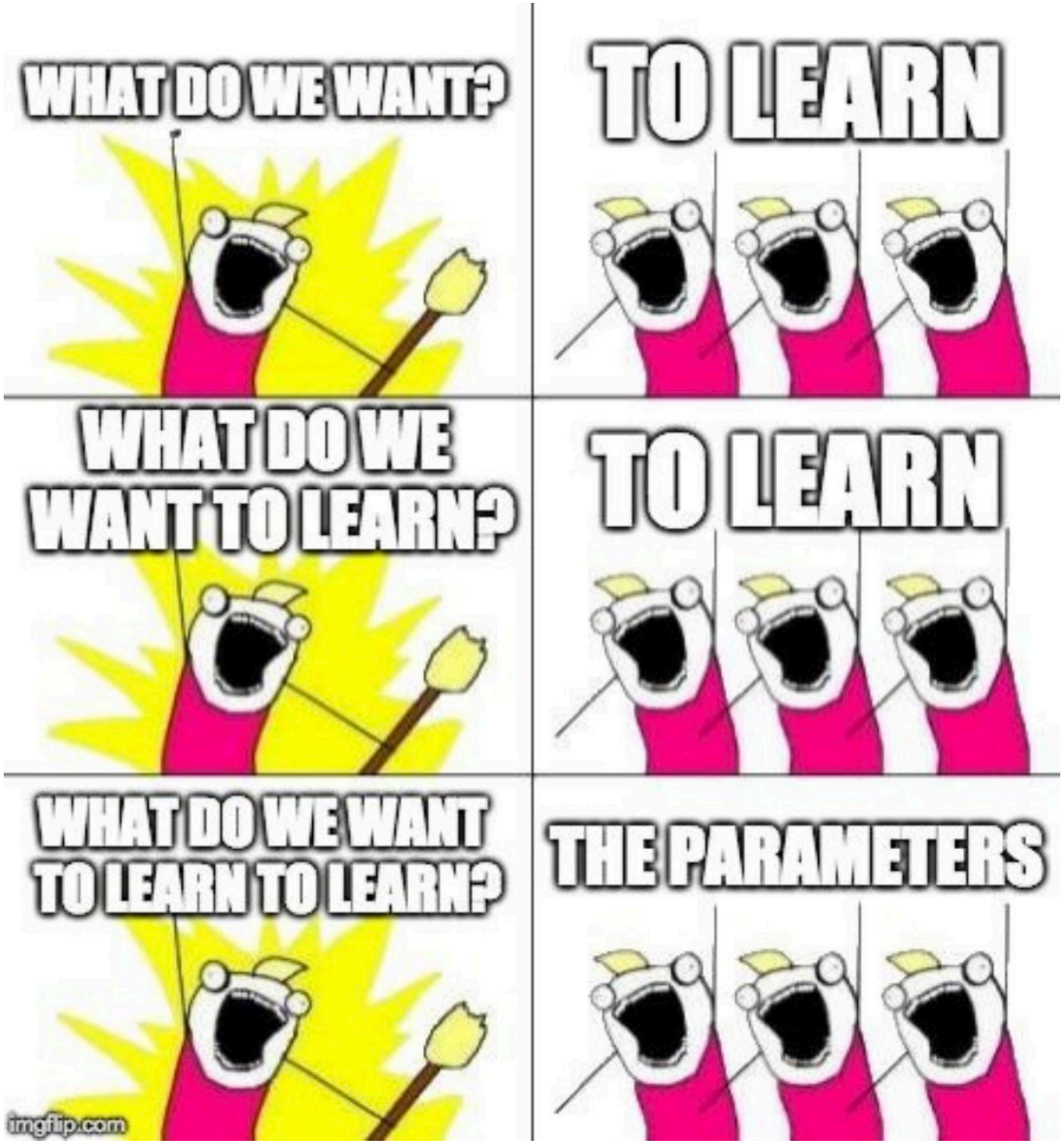


Image: Pesah et al. 2018

Andreas Mueller
Bernd Bischl
Bilge Celik
Erin LeDell
Frank Hutter
Guiseppe Casalicchio
Heidi Seibold
Jakub Smid
Jan van Rijn
Janek Thomas
Joaquin Vanschoren
Matthias Feurer
Marcel Wever
Markus Weimer
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Mitar Milutinovic
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Neil Lawrence
Pieter Gijsbers
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Sahithya Ravi
William Raynaut

Thanks to the OpenML team!

Join us :)