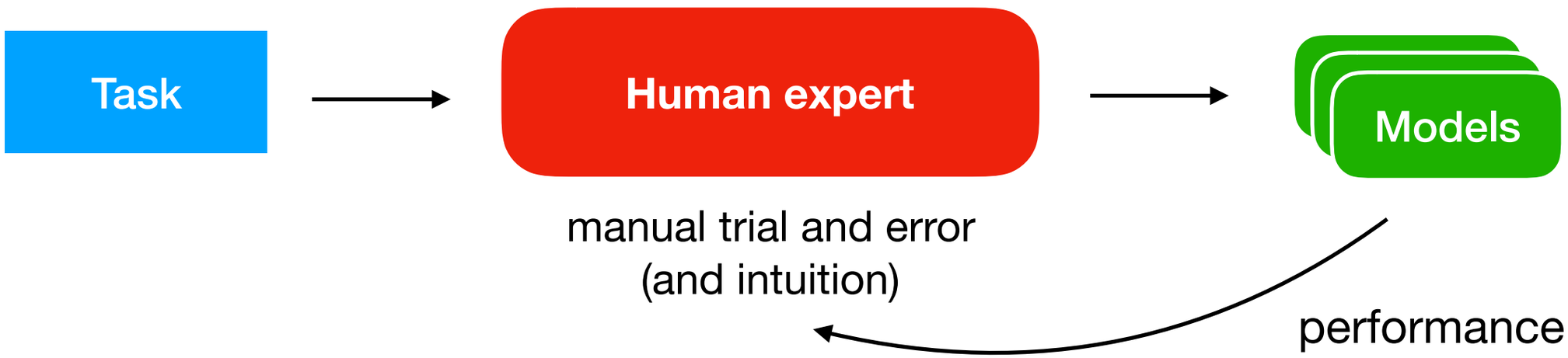
Automated Machine Learning

and learning to learn

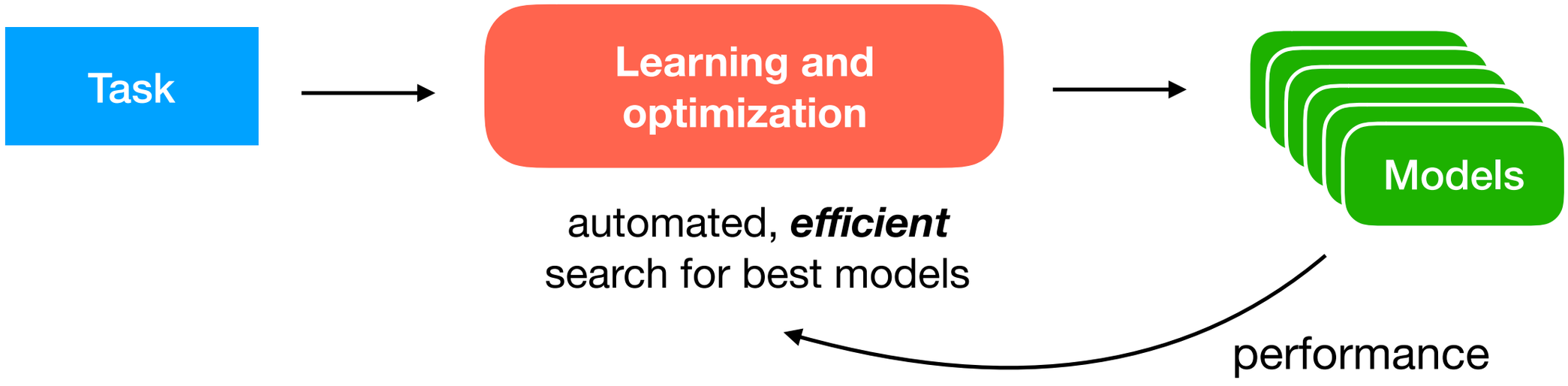
Joaquin Vanschoren, Eindhoven University of Technology

Automated Machine Learning

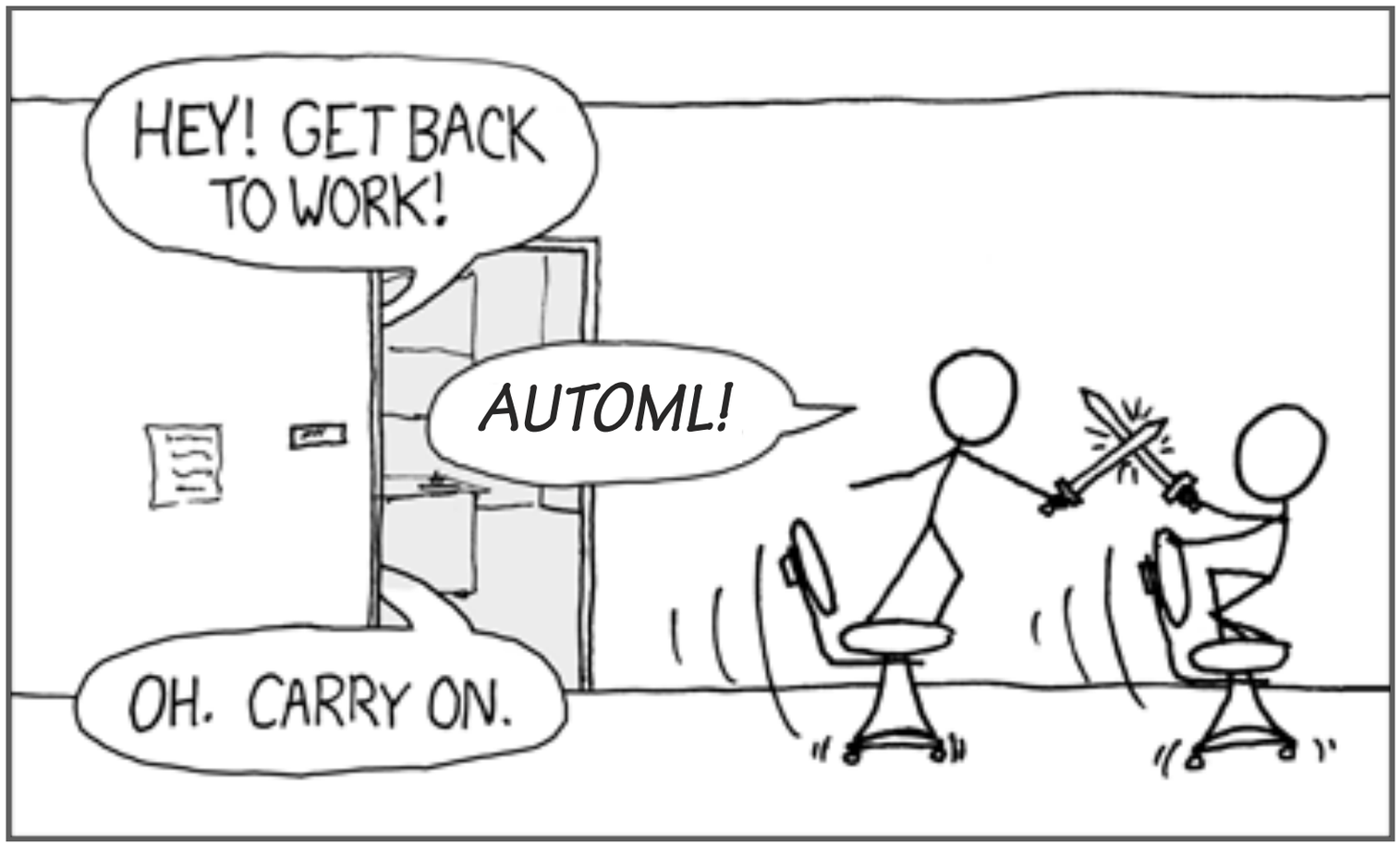
Manual machine learning



AutoML: build models in a *data-driven*, *intelligent*, *purposeful* way



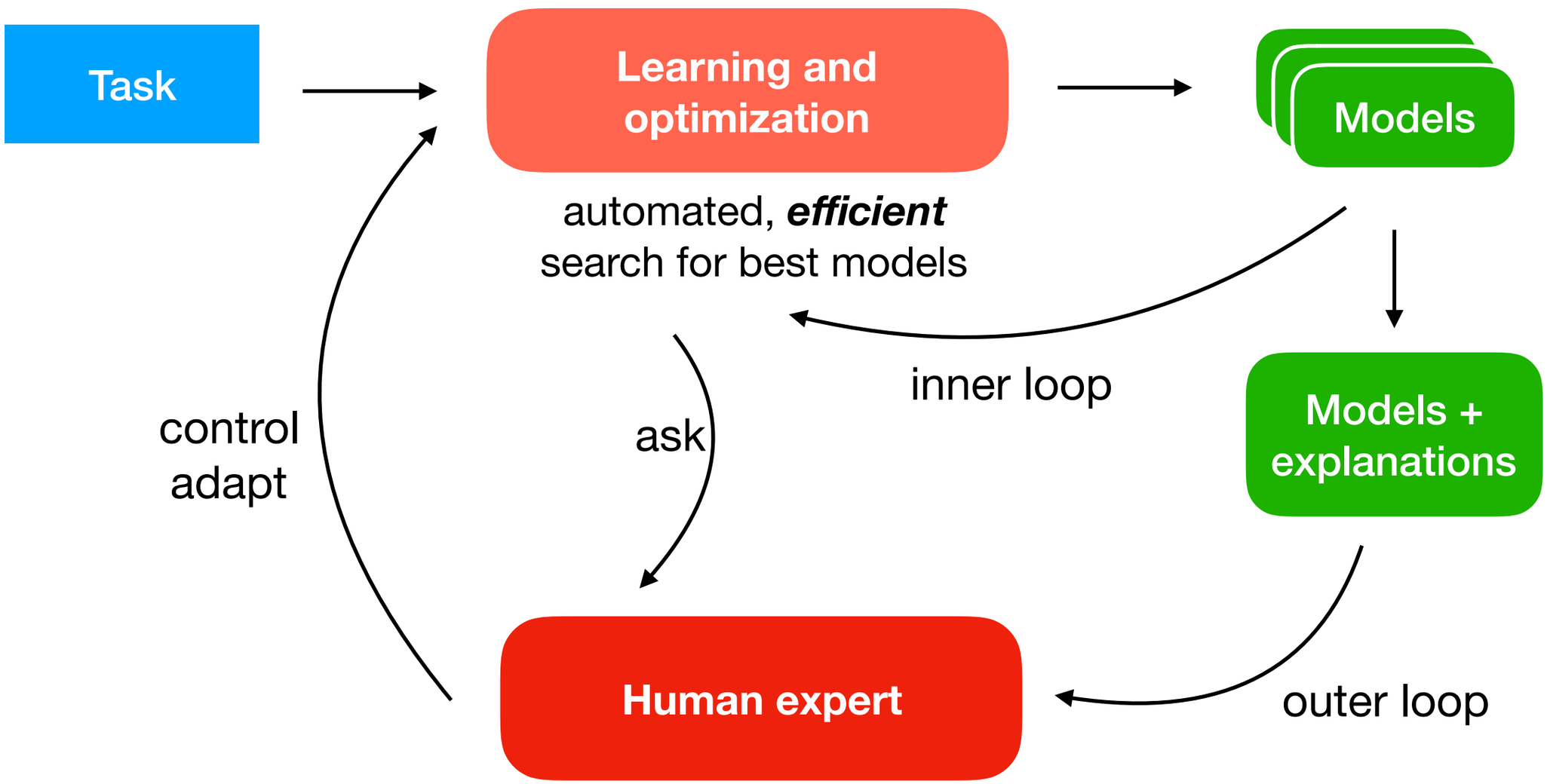
THE DATA SCIENTIST'S #1 EXCUSE FOR LEGITIMATELY SLACKING OFF: "THE AUTOML TOOL IS OPTIMIZING MY MODELS!"



Adapted from XKCD (Randall Munroe)

Semi-automated Machine Learning

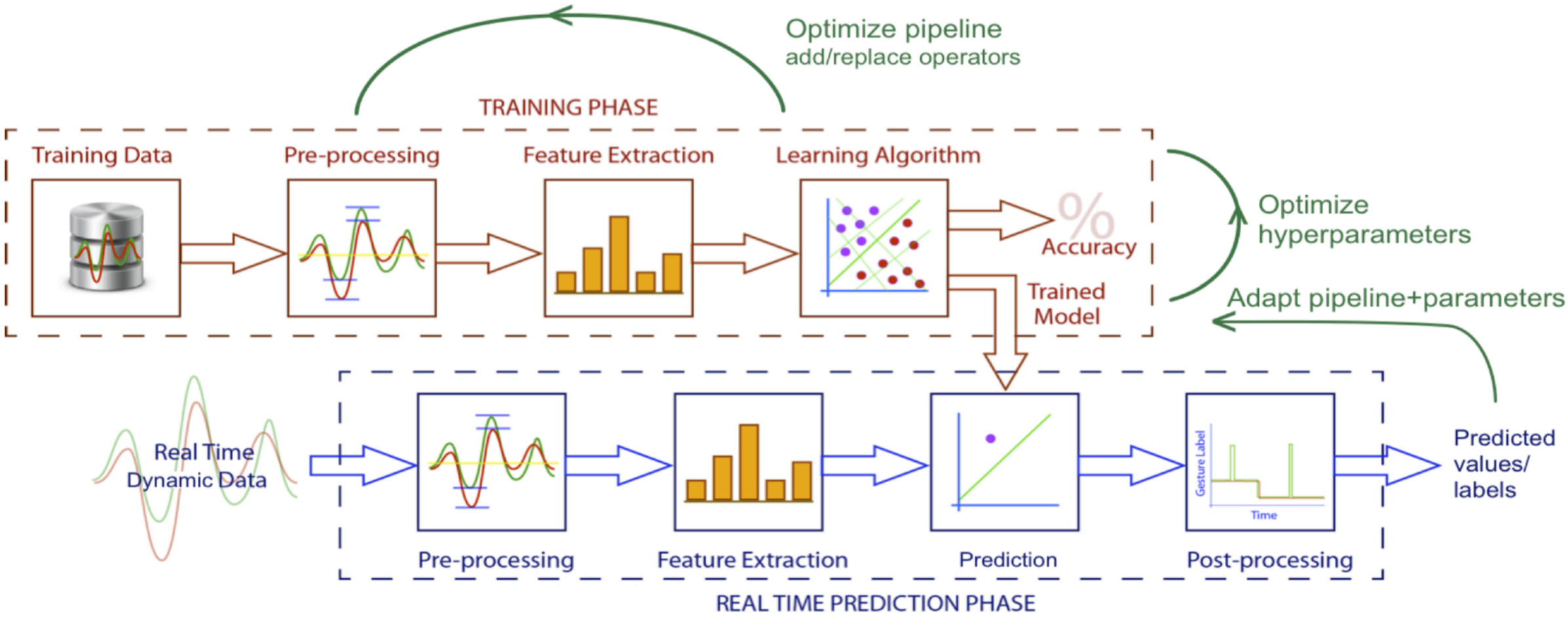
Human-in-the-loop



AutoML automates some aspects that require intelligence, but not all
Domain knowledge and human expertise remain crucial

Doing machine learning requires a lot of expertise

Pipeline synthesis



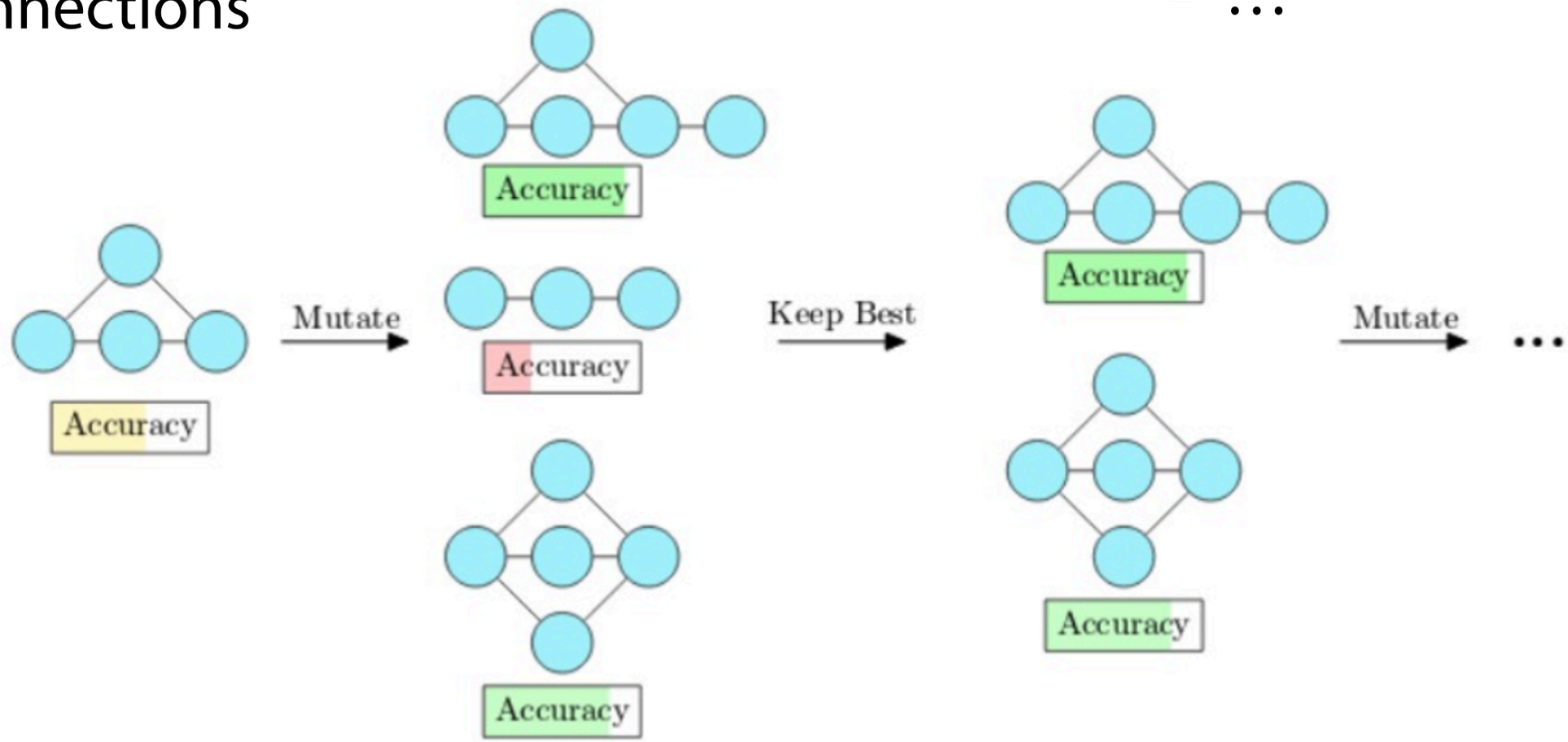
- Excellent tools (e.g. scikit-learn), but little guidance
- Cleaning, preprocessing, feature selection/engineering features, model selection, hyperparameter tuning, adapting to concept drift,…

Doing machine learning requires a lot of expertise

Neural Architecture Search (NAS)

- Type of operators
- Size of layers
- Filter sizes
- Skip connections
- …

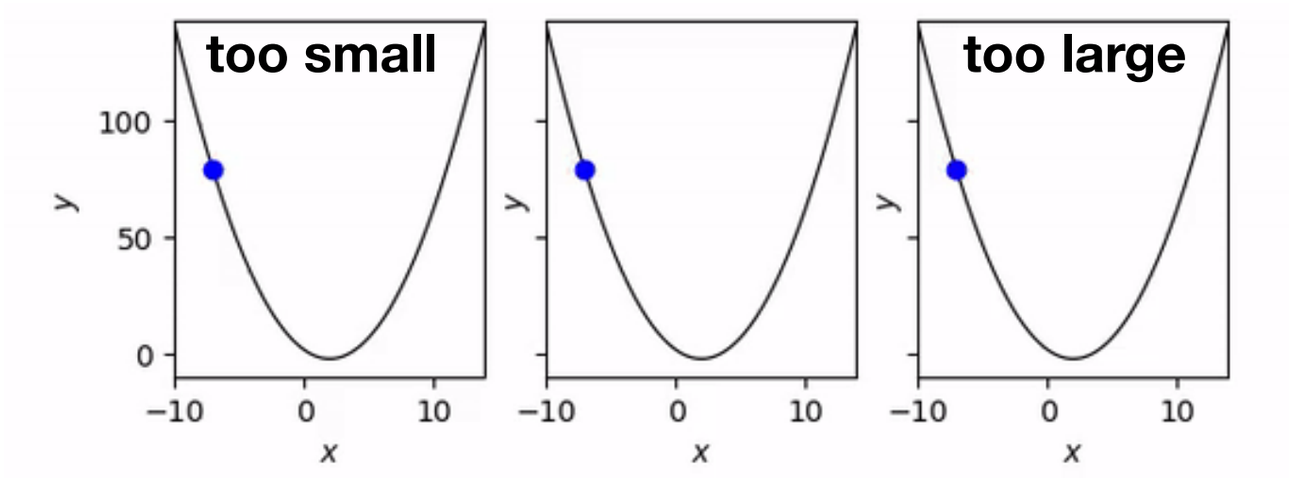
- Gradient descent hyperparameters
- Regularization
- …



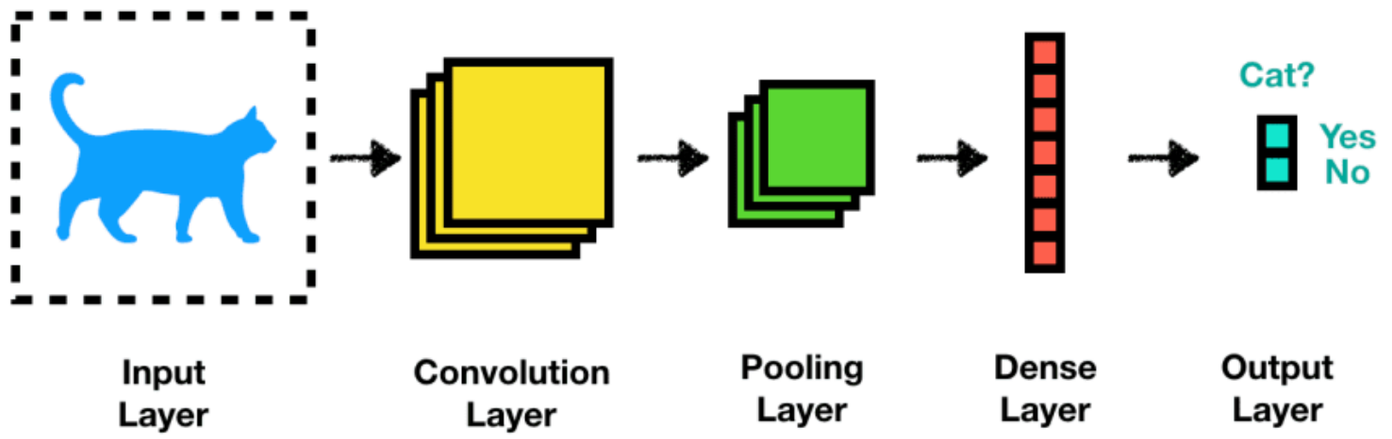
Hyperparameters

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

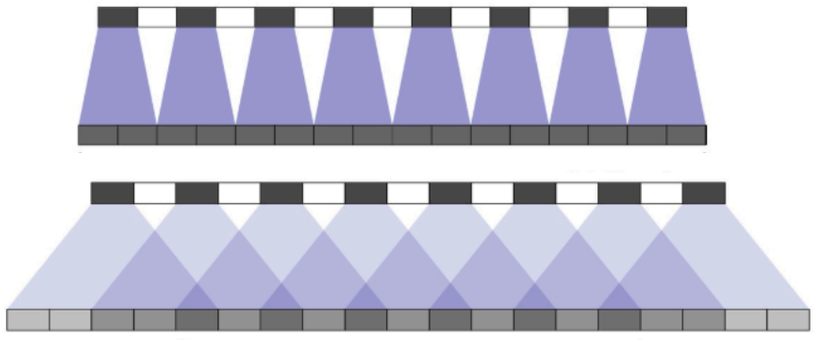
- Numeric
  - e.g. learning rate



- Categorical
  - e.g. layer type



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



Filter size 2, stride length 2

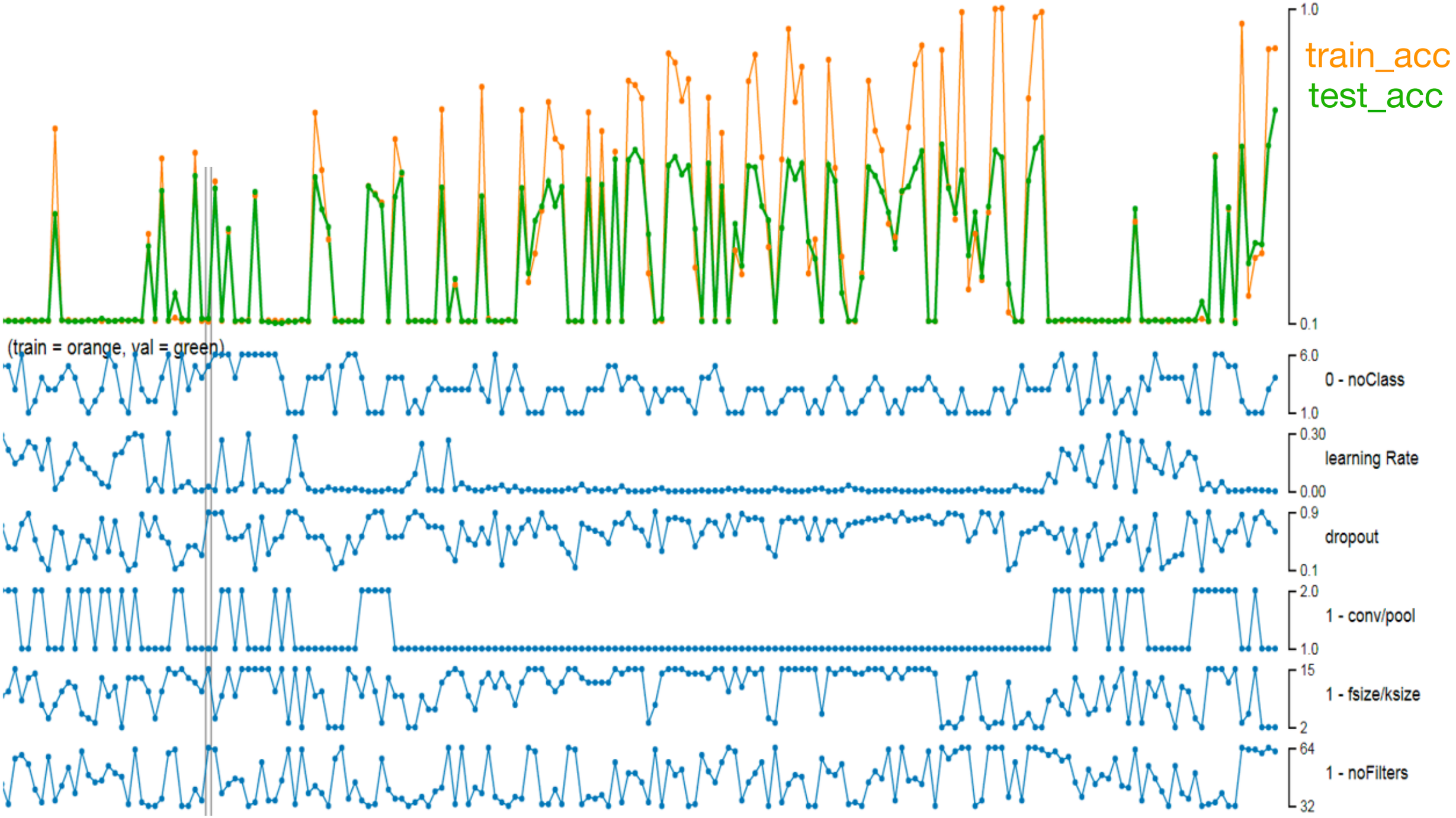
Filter size 5, stride length 2

Hyperparameters

Some are very sensitive, others not. Many interact.

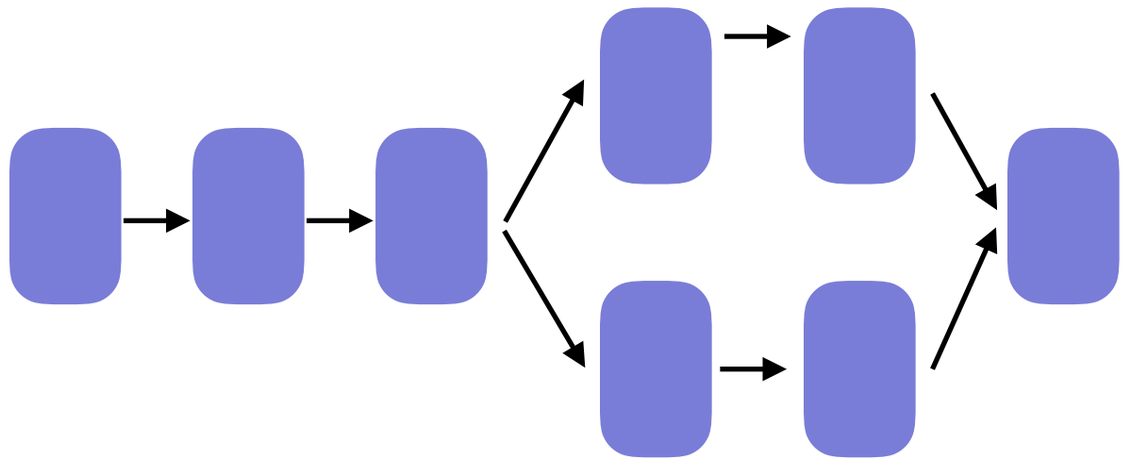
What is the right strategy to find the right ***configuration***?

Can we do better than random search?



AutoML: subproblems

- **Architecture search**: *represent* and *search* all pipelines or neural nets
  - Pipeline operators, neural layers, interconnections,…
  - Defines the search space

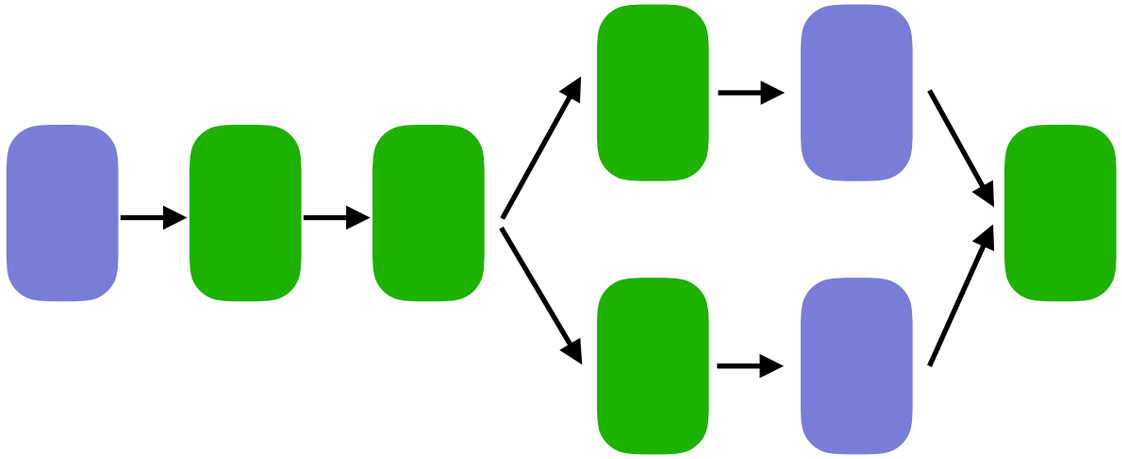


```
make_pipeline(
  OneHotEncoder(),
  Imputer(),
  StandardScaler(),
  SVC())
```

```
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

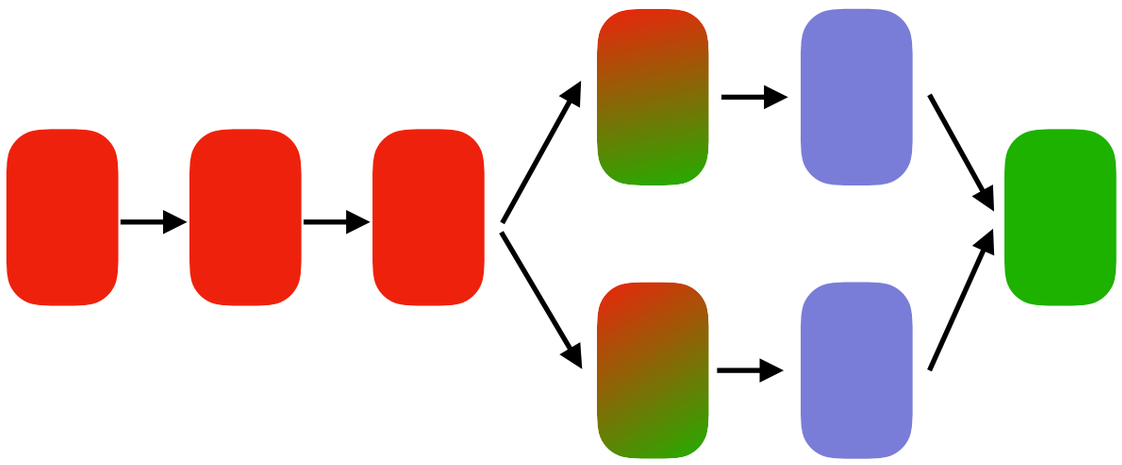
- **Architecture search**: *represent* and search all possible architectures
- **Hyperparameter optimization**:
  - Which hyperparameters are important? How to optimize them?
  - What is the (multi-)objective function?



```
def build_model(hp){
    m.add(Dense(units=hp.Int('units', min_value=32, max_value=512, step=32)))
    m.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* remaining hyperparameters
- **Meta-learning**: how can we transfer *experience* from previous tasks?
  - Don't start from scratch (search space is too large)



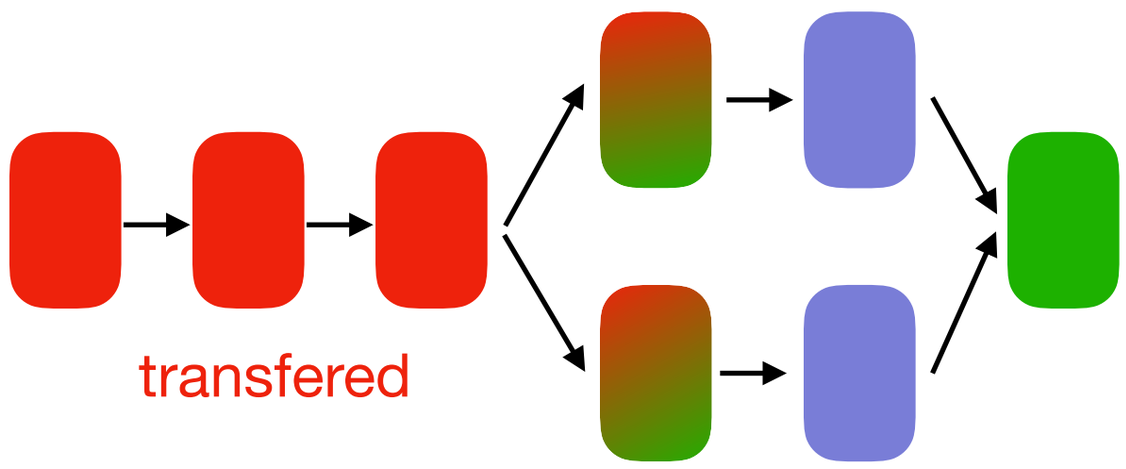
Goal:

```
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* important hyperparameters
- **Meta-learning**: how can we transfer experience from previous tasks?
  - Transfer learning: reuse good architectures/configurations
  - Warm starting: start from promising architectures/configurations
  - …



AutoML: subproblems

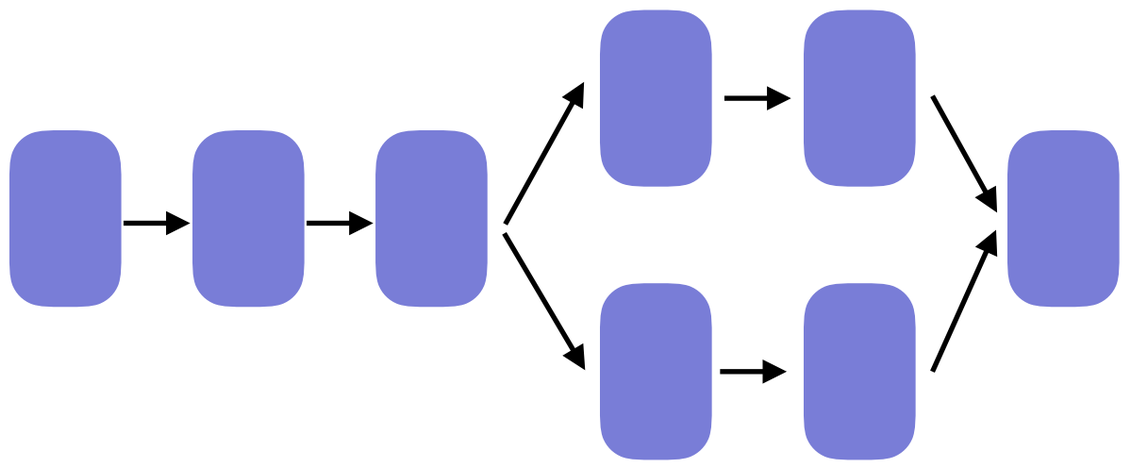
- **Architecture search**: *represent* and search all possible architectures
- **Hyperparameter optimization**: *optimize* remaining hyperparameters
- **Meta-learning**: how can we transfer experience from previous tasks?

Many combinations are possible!
They can be done *consecutively*, *simultaneously* or *interleaved*

So… yeah, this is a meta-meta-learning problem

AutoML: subproblems

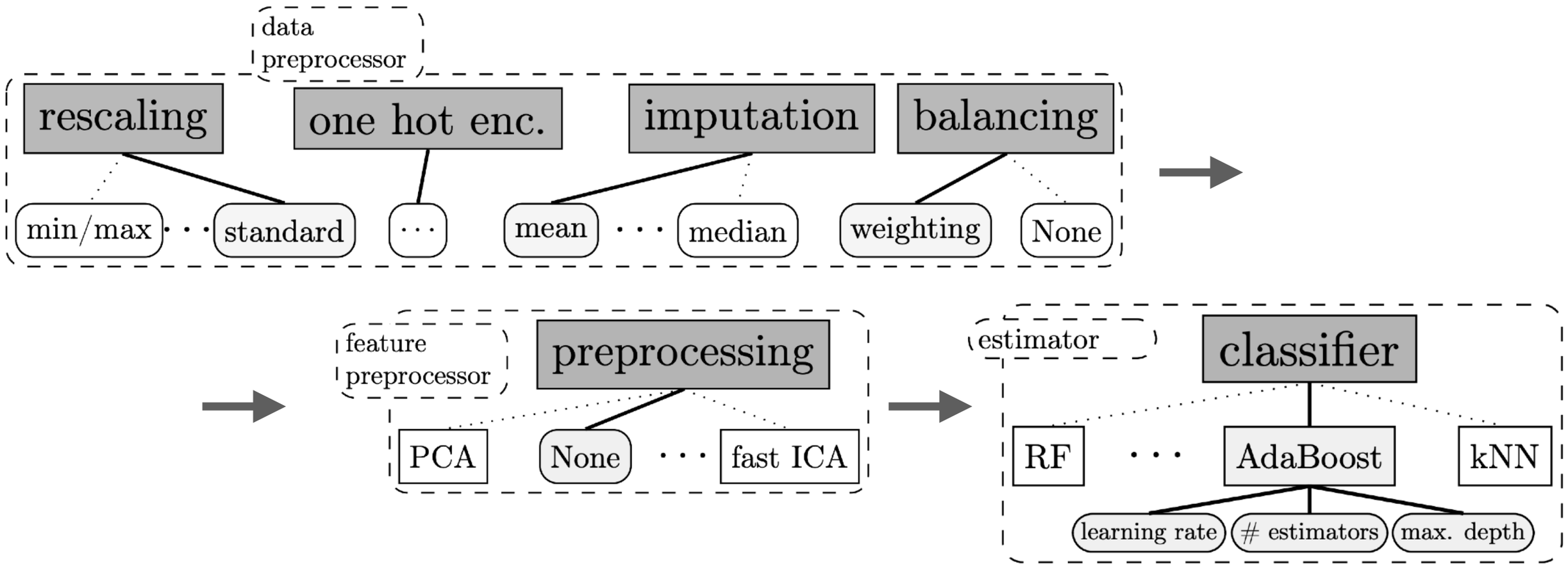
- **Architecture search**: *many different approaches*
  - Parameterized (fixed) architectures
  - Reinforcement learning
  - Evolution
  - Heuristic search
  - …



autosklearn *Feurer et al. 2015*
autoWEKA *Thornton et al. 2013*
hyperopt-sklearn *Komer et al. 2014*

Parameterized architecture

- From experience: most successful pipelines have a similar structure
- Fix architecture, encode all choices as extra hyperparameters
  - *Architecture search becomes hyperparameter optimization*



+ smaller search space
- you can't learn entirely new architectures

Elsken et al. 2019

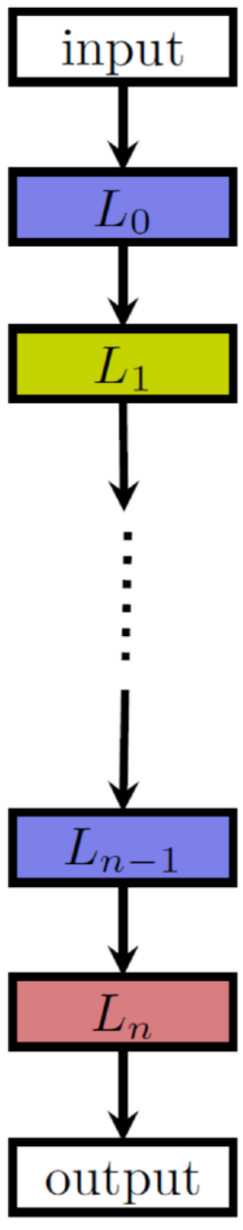
Parameterized neural architectures

Parameterized Sequential

Choose:

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

+ easier to search
- sometimes too simple

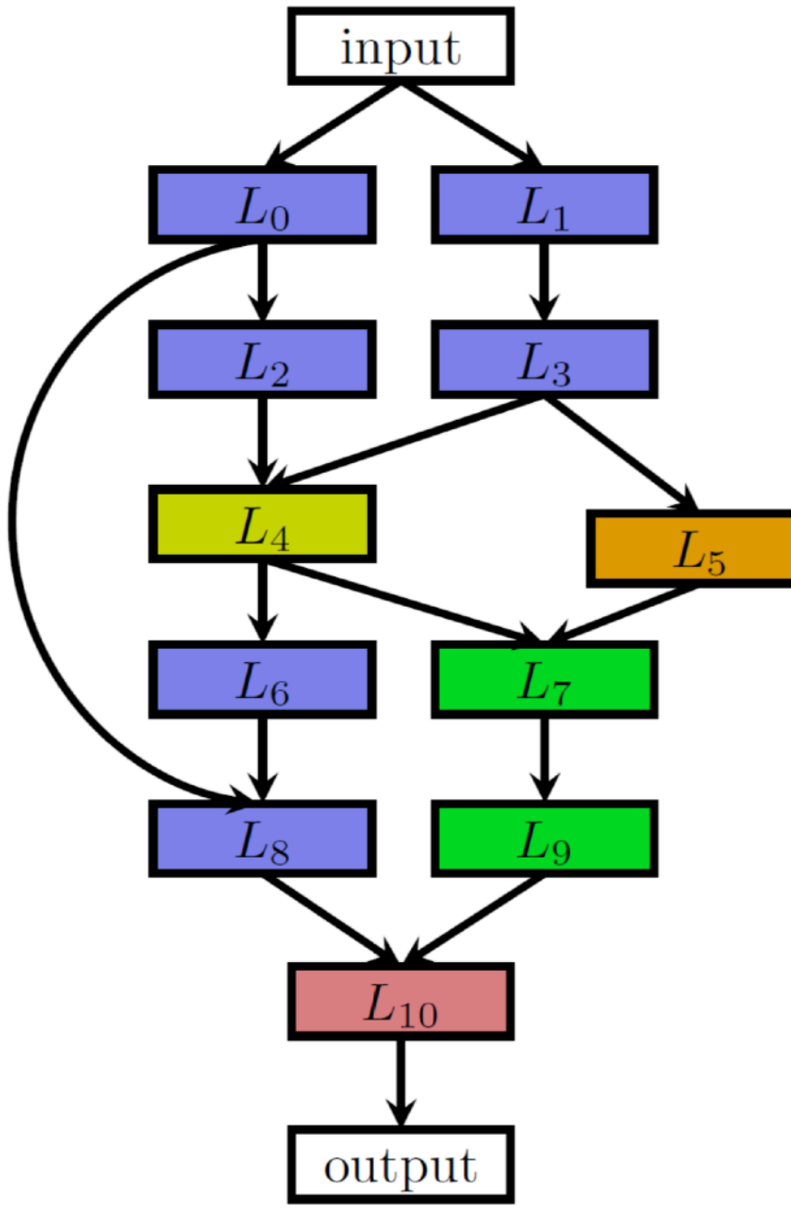


Parameterized Graph (Hypernetwork)

Choose:

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

+ more flexible
- much harder to search

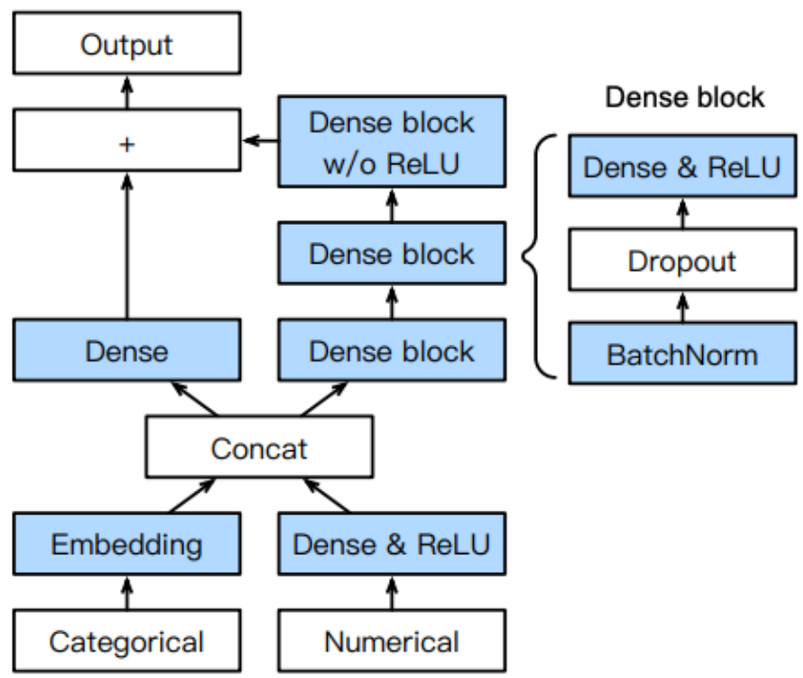


Erickson et al 2020

Fusi et al. 2017

Portfolios

- From experience: Some subsets of models that often work well
- Choose a set (portfolio) of models, and then tune them to the new task
  - Beneficial when there are strong time constraints
- Examples:
  - *PMF (Microsoft AutoML)*: 1000s of pipelines + meta-model
  - *Amazon AutoGluon*: Boosting (2x), RandomForests, kNN, TabularNN
    - With ensembling of best models

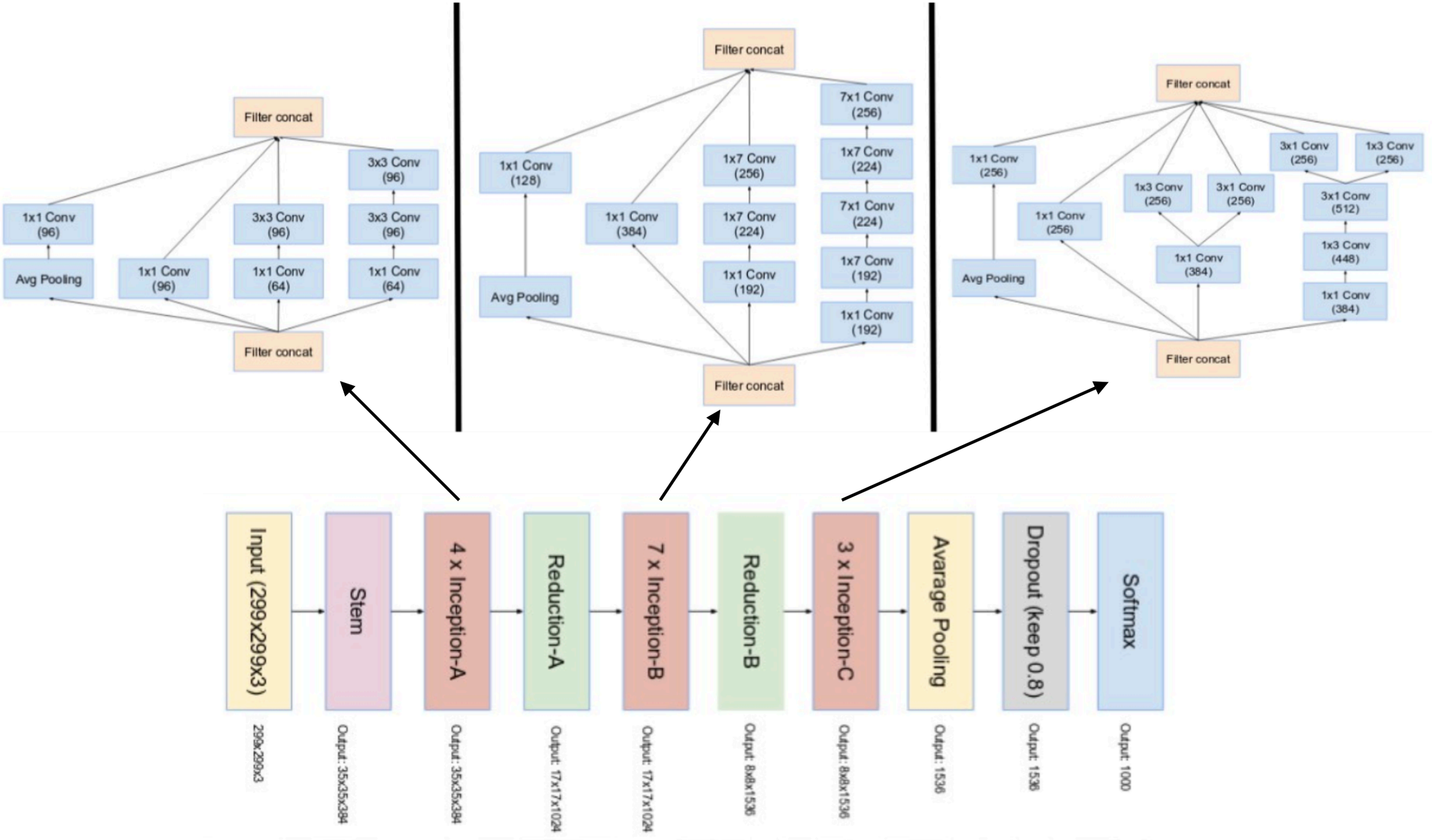


Neural network for tabular data
(trainable layers in blue)

Neural Architecture Search

From experience: successful deep networks have repeated motifs (cells)

e.g. Inception v4:



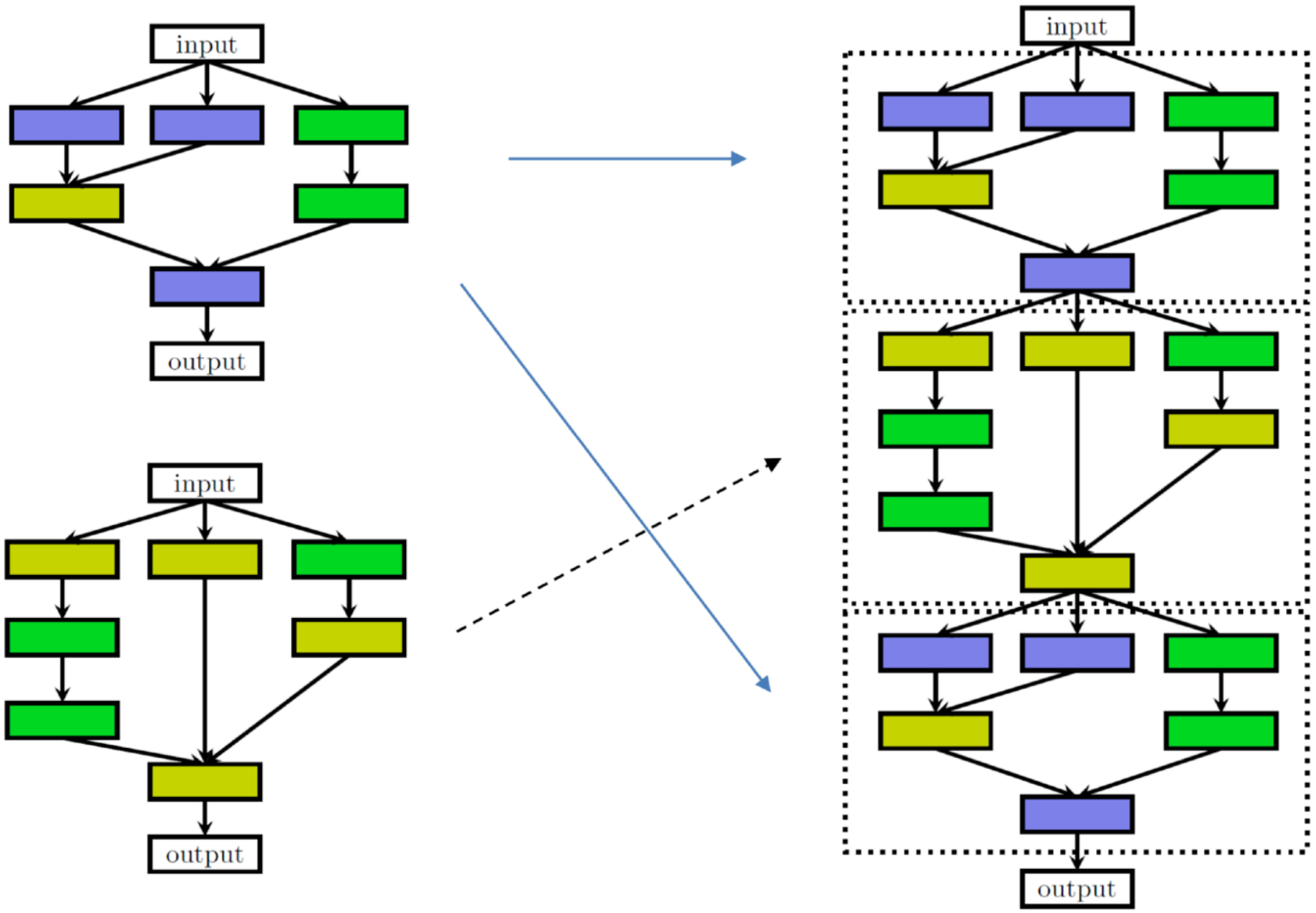
Google NASNet Zoph et al 2018

Meta-architectures

Compositionality: learn hierarchical building blocks to simplify the task

Cell search space

- learn parameterized building blocks *(cells)*
- stack cells together in macro-architecture

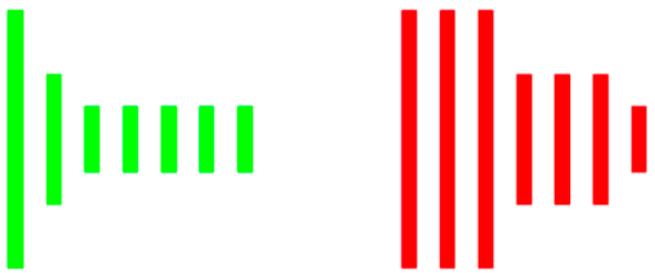


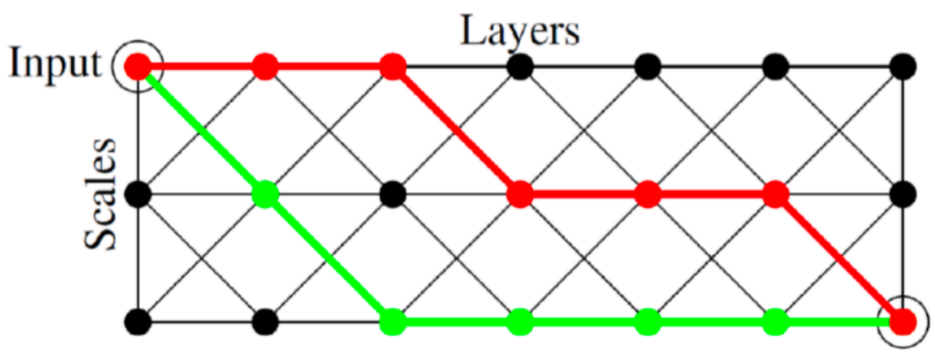
+ smaller search space
+ cells can be learned on a small dataset & transferred to a larger dataset
− strong domain priors, doesn't generalize well

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

Hypernetworks

- Every candidate network belongs to a *hypernetwork*



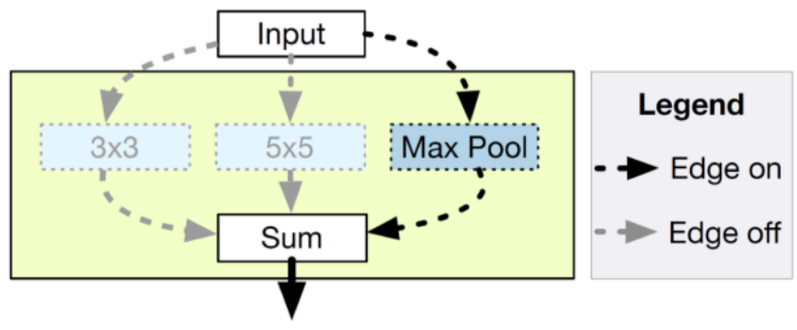


'Neural fabric' for 7-layer CNNs with differing feature map sizes[1]

  - Train in parallel, share the (filter) weights of 'common' layers: faster
    - Hypernetwork can be designed to reduce the search space

- *EfficientNAS* [2]
  - use RL to sample paths from the hypernetwork graph, share weights

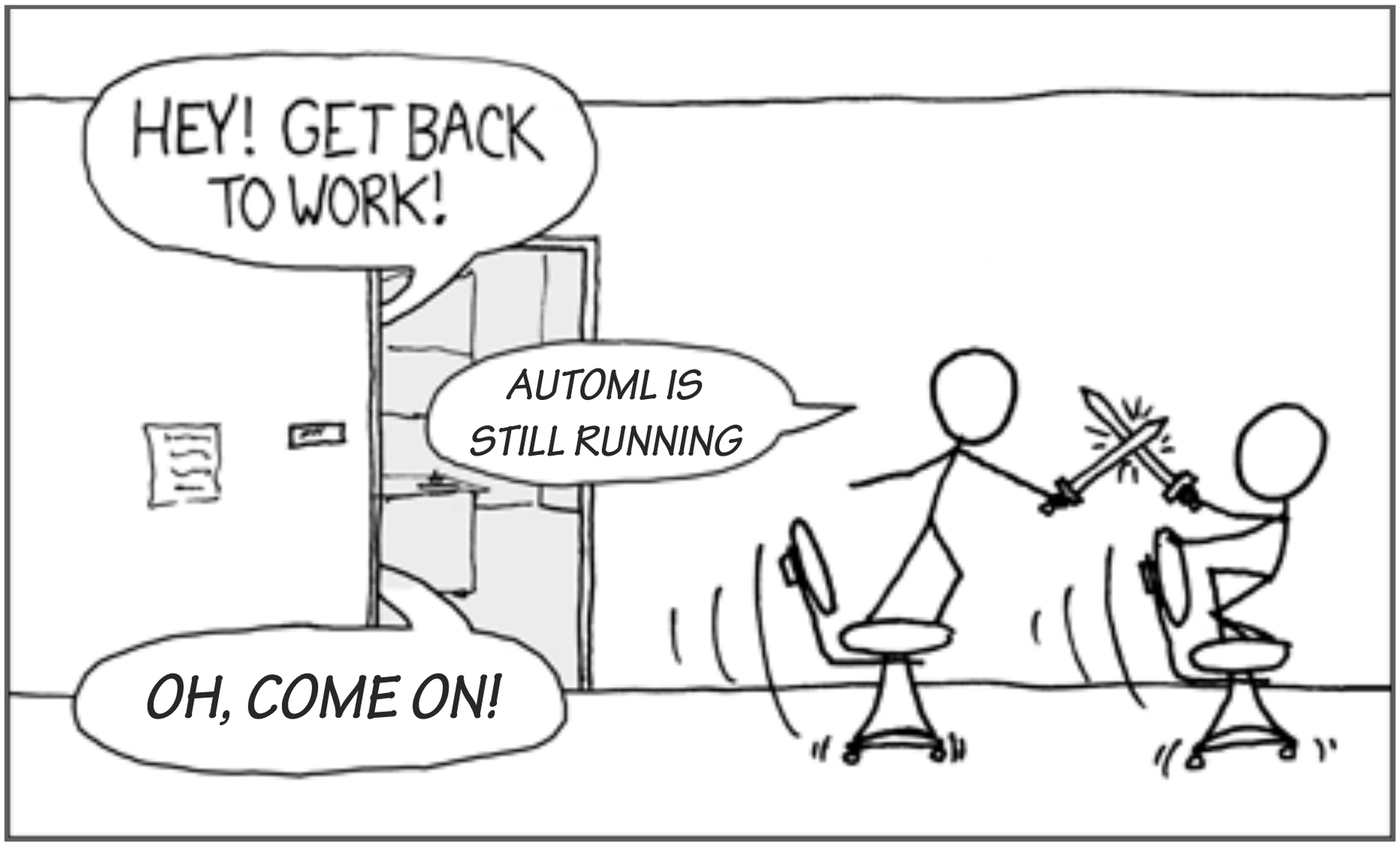
- *One-shot models* [3]
  - Train all nets in parallel, with *path dropout*



- *SMASH* [4]
  - Learns meta-model that predicts good model weights given architecture

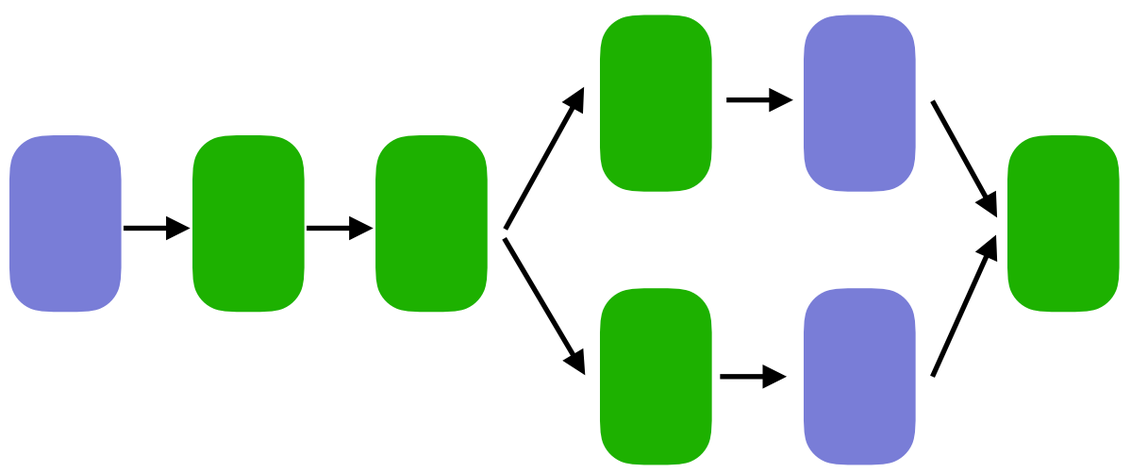
Hyperparameter Optimization

Searching the hyperparameter space ***efficiently***



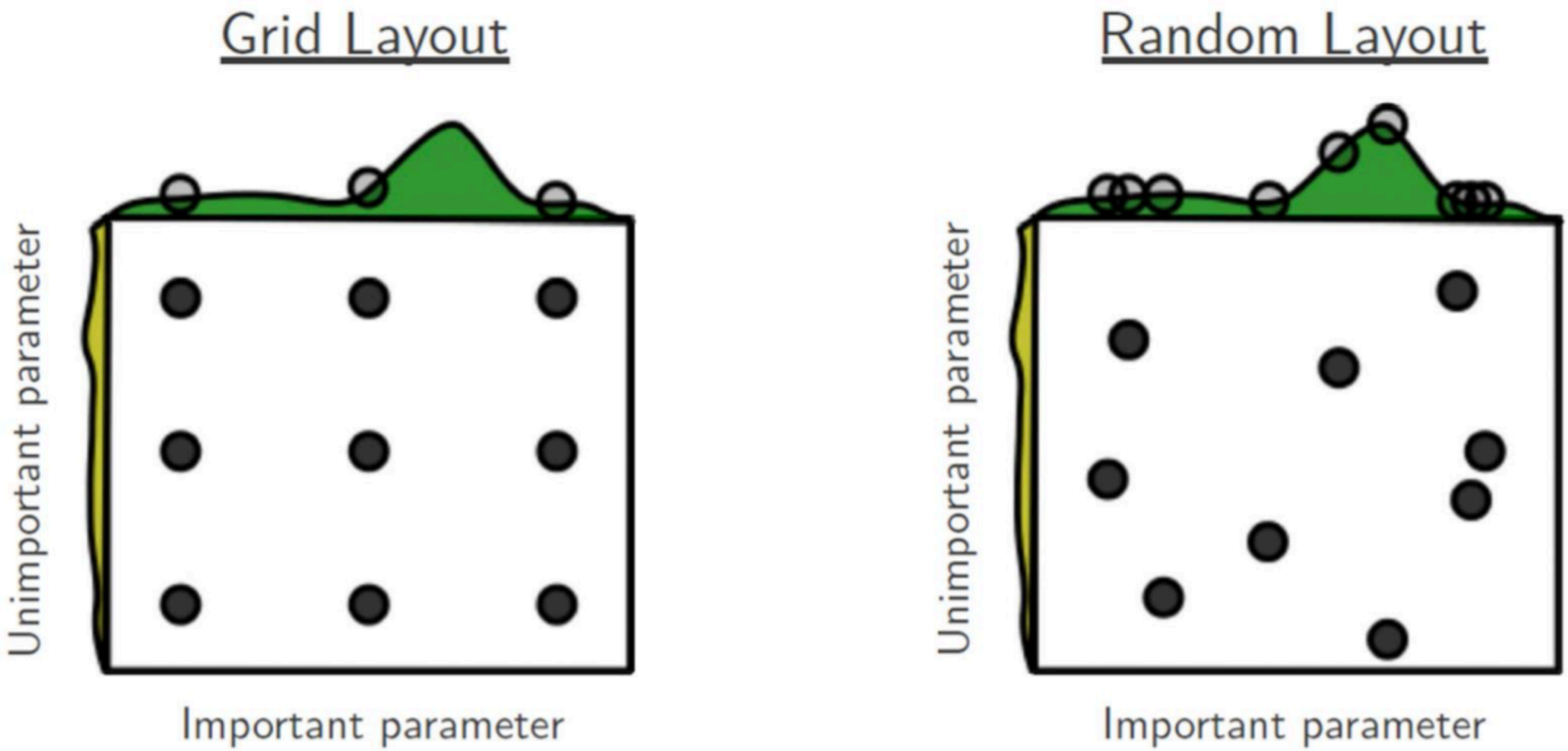
AutoML: subproblems

- **Hyperparameter optimization**: *many different approaches (and tools!)*
  - 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

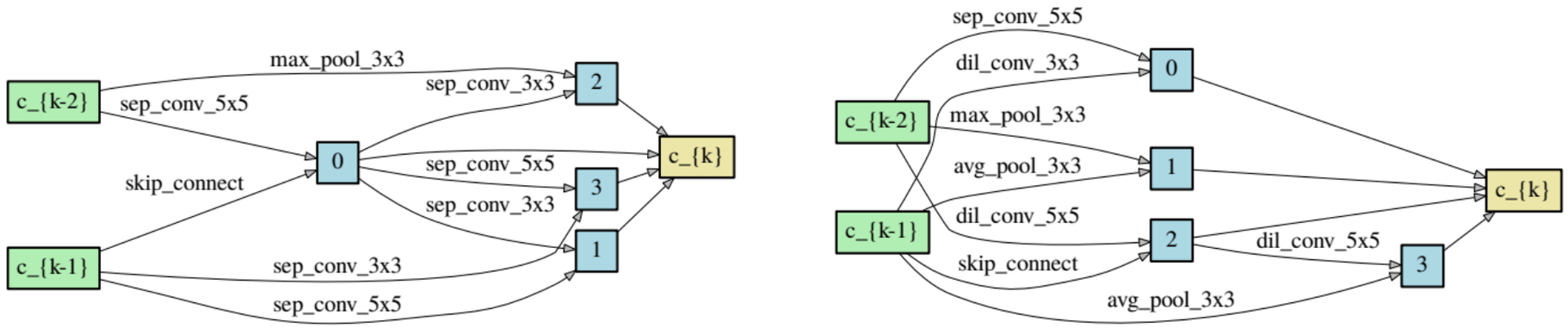
Random search

Li & Talwalkar 2019

Yu et al. 2019

Real et al. 2019

Neural Architecture search: if you constrain the search space enough, you can get SOTA results with random search! E.g.: with cell search space:



(a) Normal Cell (b) Reduction Cell

Convolutional Cells on CIFAR-10 Benchmark: Best architecture found by random search with weight-sharing.

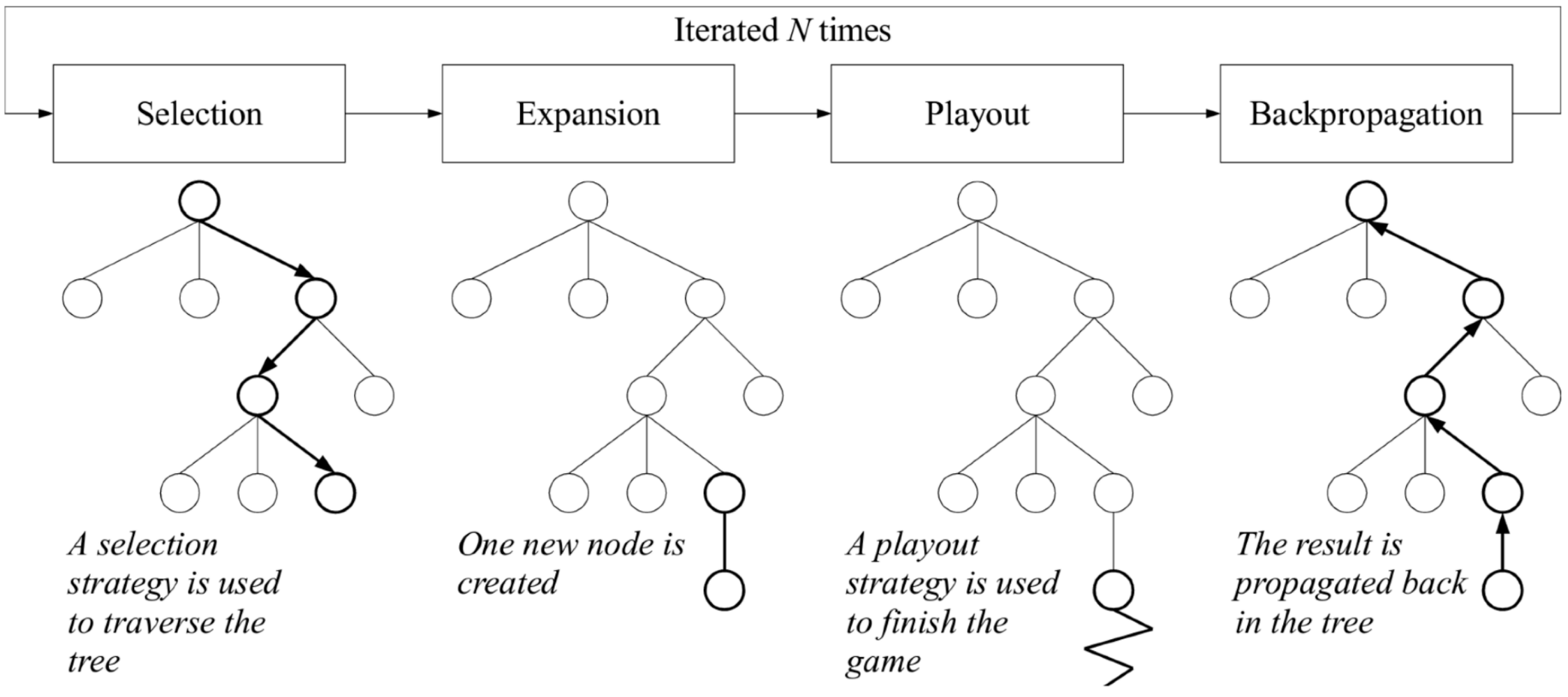
H2O AutoML: Runs random search over parameterized pipelines and then stacks the trained models

```
# Run AutoML for 20 base models (limited to 1 hour max runtime by default)
aml = H2OAutoML(max_models=20, seed=1)
aml.train(x=x, y=y, training_frame=train)

# AutoML Leaderboard
lb = aml.leaderboard
```

MOSAIC [Rakotoarison et al. 2019]
AlphaD3M [Drori et al. 2018]

Heuristic Search

- Monte Carlo Tree Search (MCTS)
  - Select partial pipeline from tree of all pipelines
  - Add one new operator, do random completion to estimate accuracy
  - Update nodes according to performance

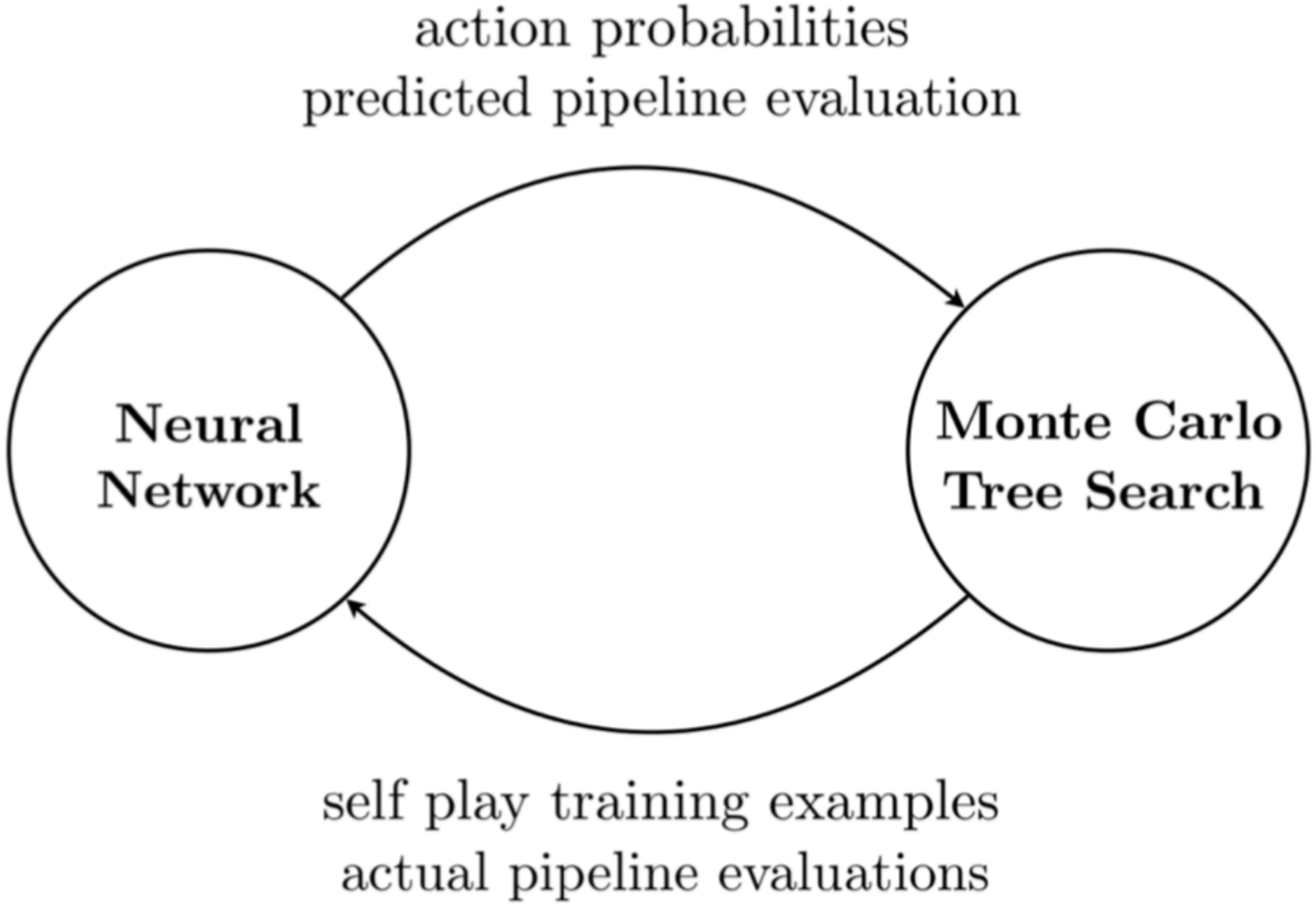


[Chaslot et al., 2008]

MOSAIC [Rakotoarison et al. 2019]
AlphaD3M [Drori et al. 2018]

Heuristic Search

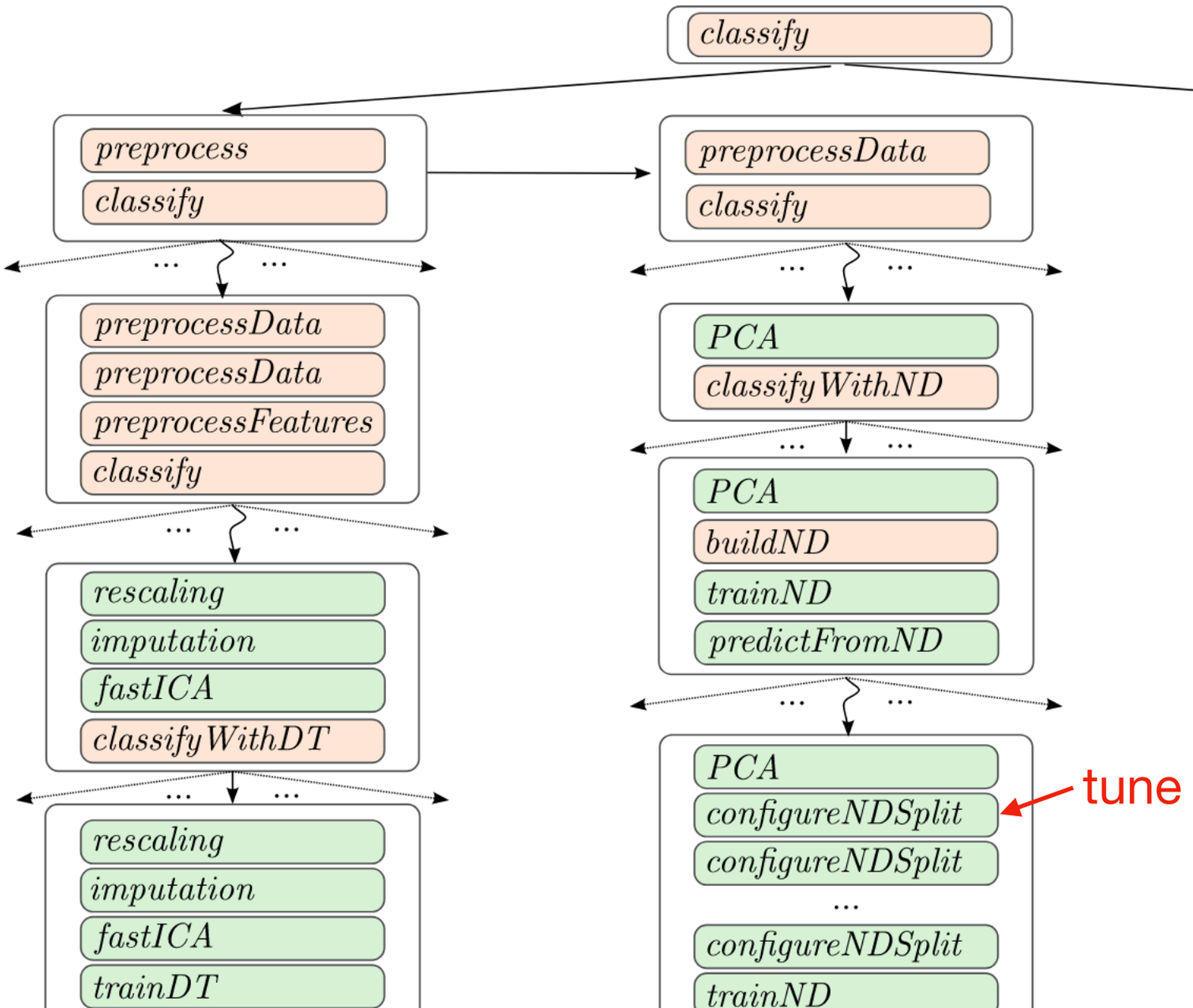
- Use reinforcement learning (RL) agent to predict good ways to extend the architecture
  - Build pipelines by inserting, deleting, replacing components (actions)
- Train the RL agent through *self-play:*
  - Monte Carlo Tree Search builds pipelines given action probabilities
  - Neural network (LSTM) Predicts pipeline performance



ML-Plan [Mohr et al. 2018]
P4ML [Gil et al. 2018]

Heuristic Search

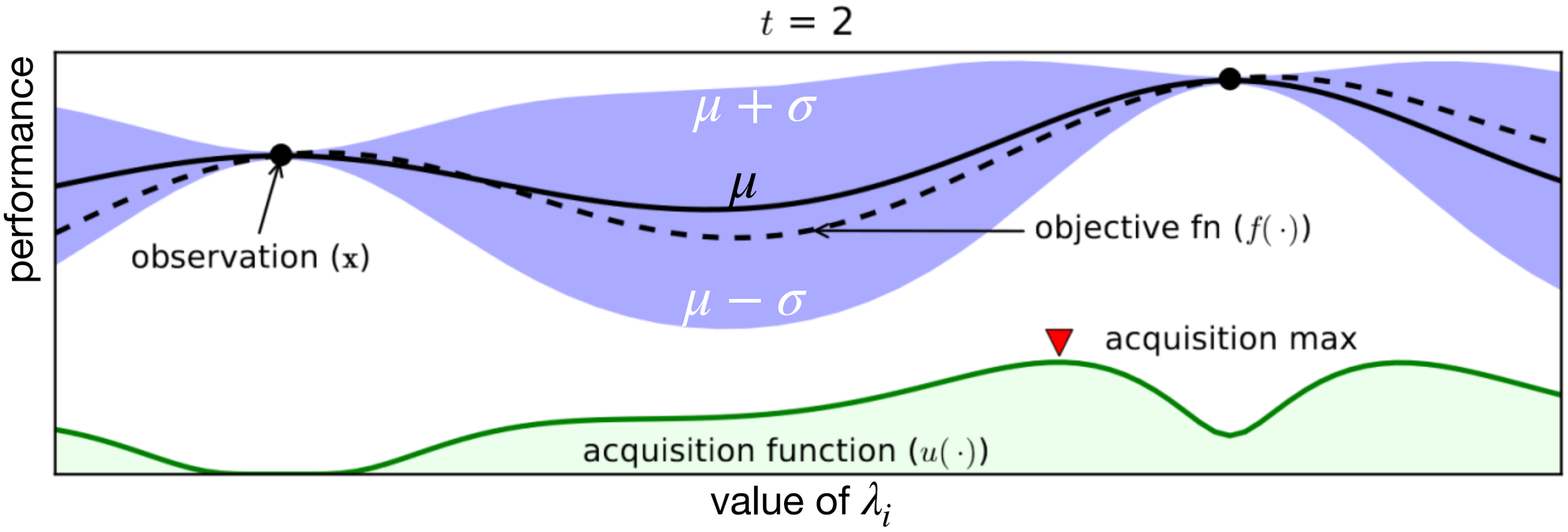
- Hierarchical planning algorithms to ‘plan' pipeline (best first search)
- Use random path completion (as in MCTS) to evaluate each node



Mockus [1974]

Bayesian Optimization

- Start with a few (random) hyperparameter configurations for hyperparameter λ_i
- 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



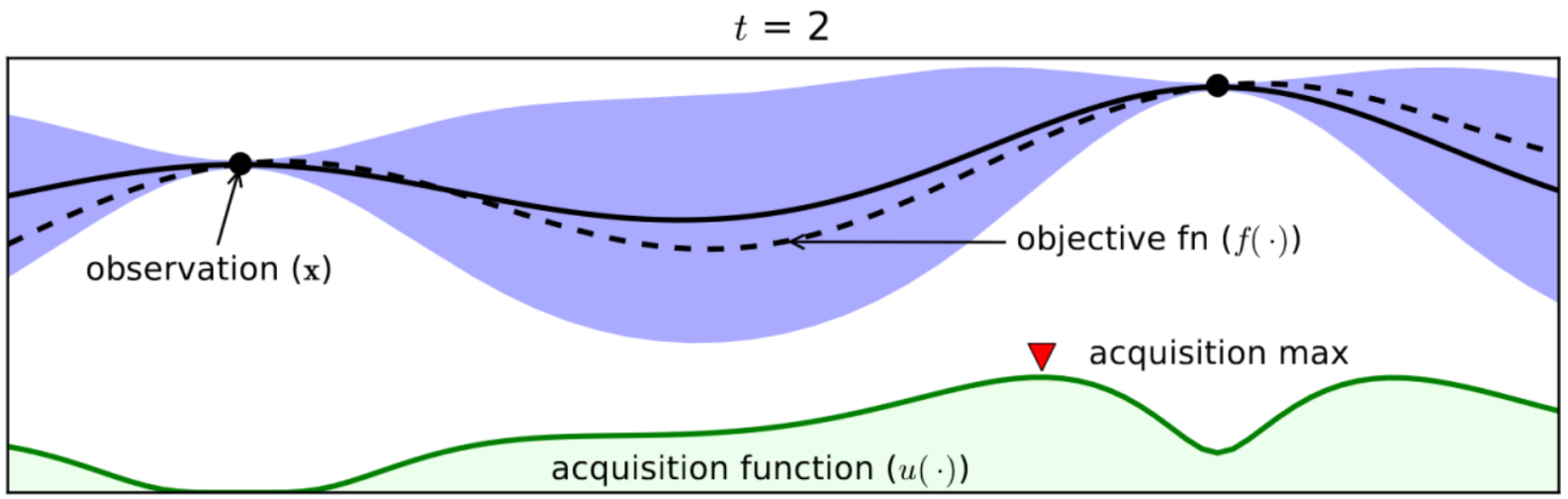
Hyperparameter optimization

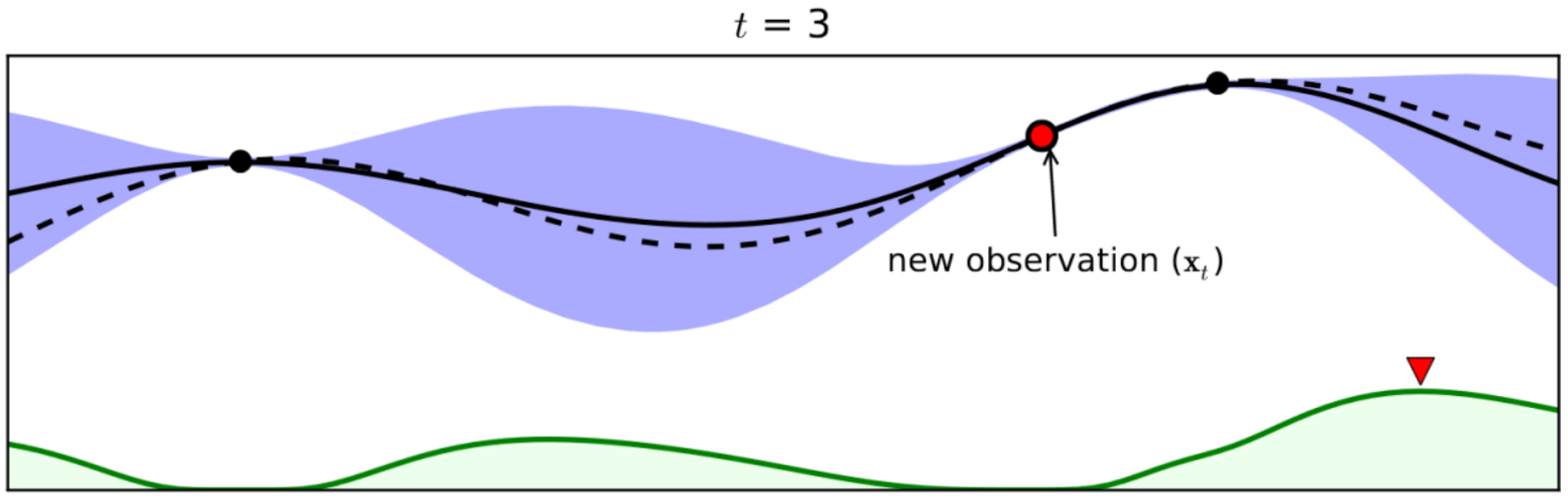
Bayesian Optimization

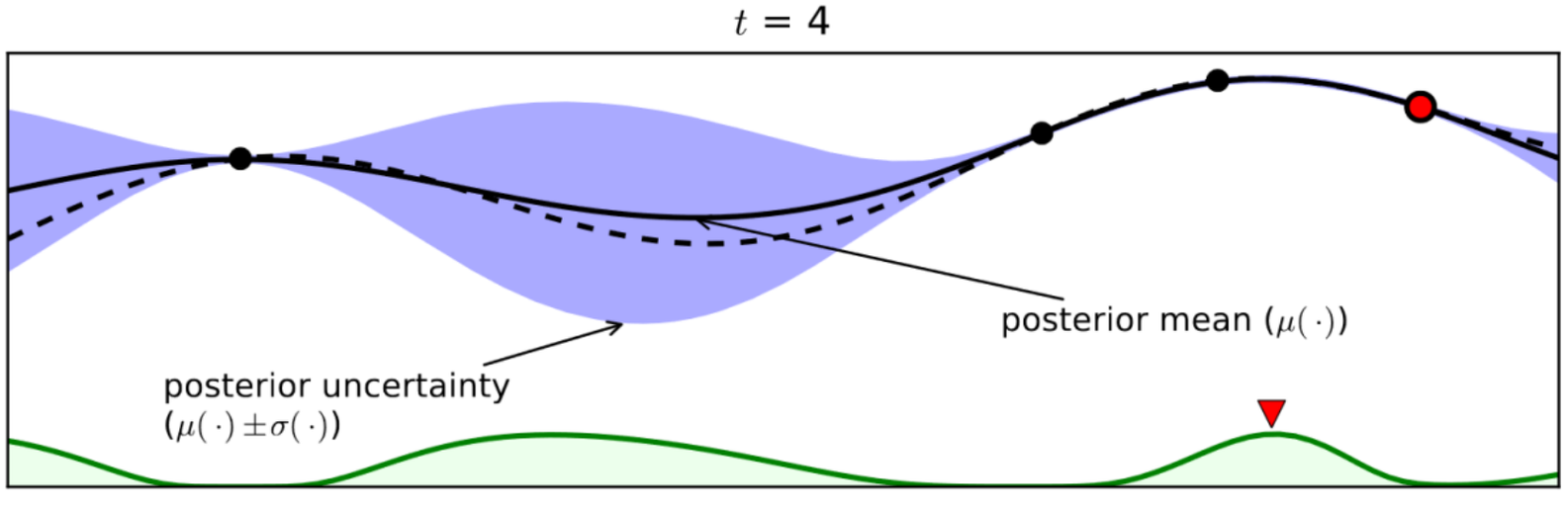
- Repeat until some stopping criterion:
  - Fixed budget
  - Convergence
  - EI threshold

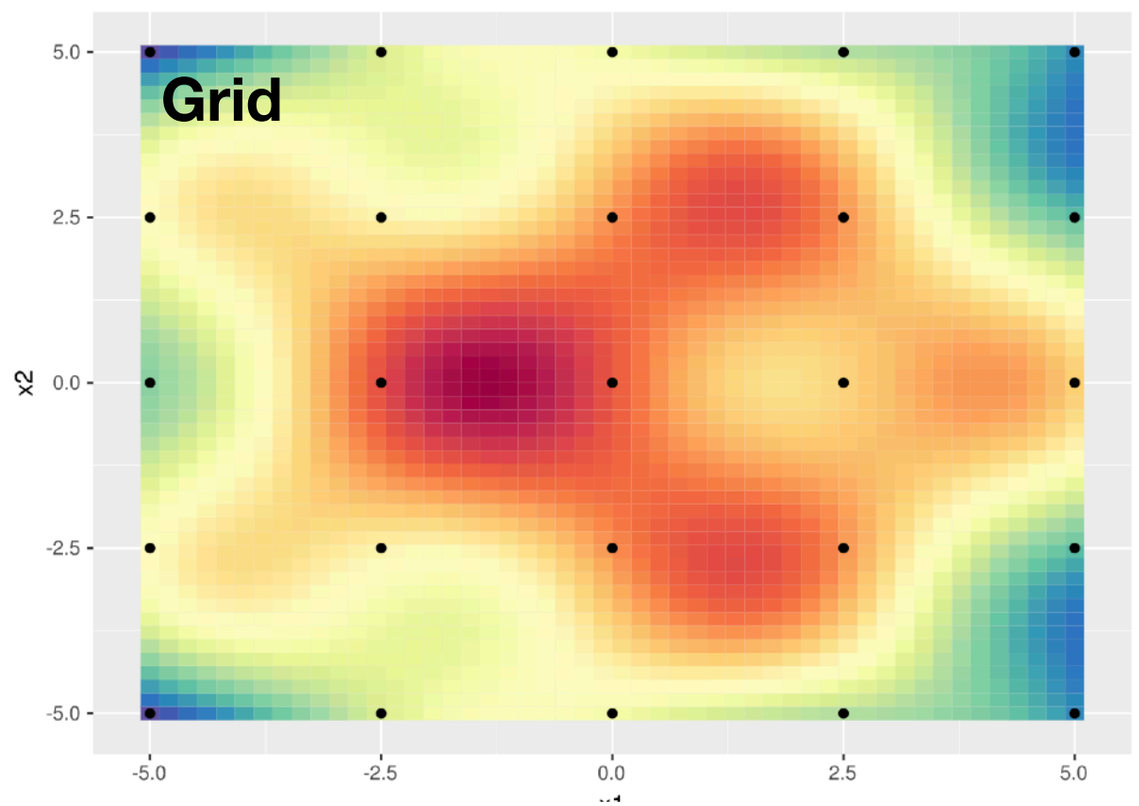
- Theoretical guarantees
  Srinivas et al. 2010, Freitas et al. 2012, Kawaguchi et al. 2016

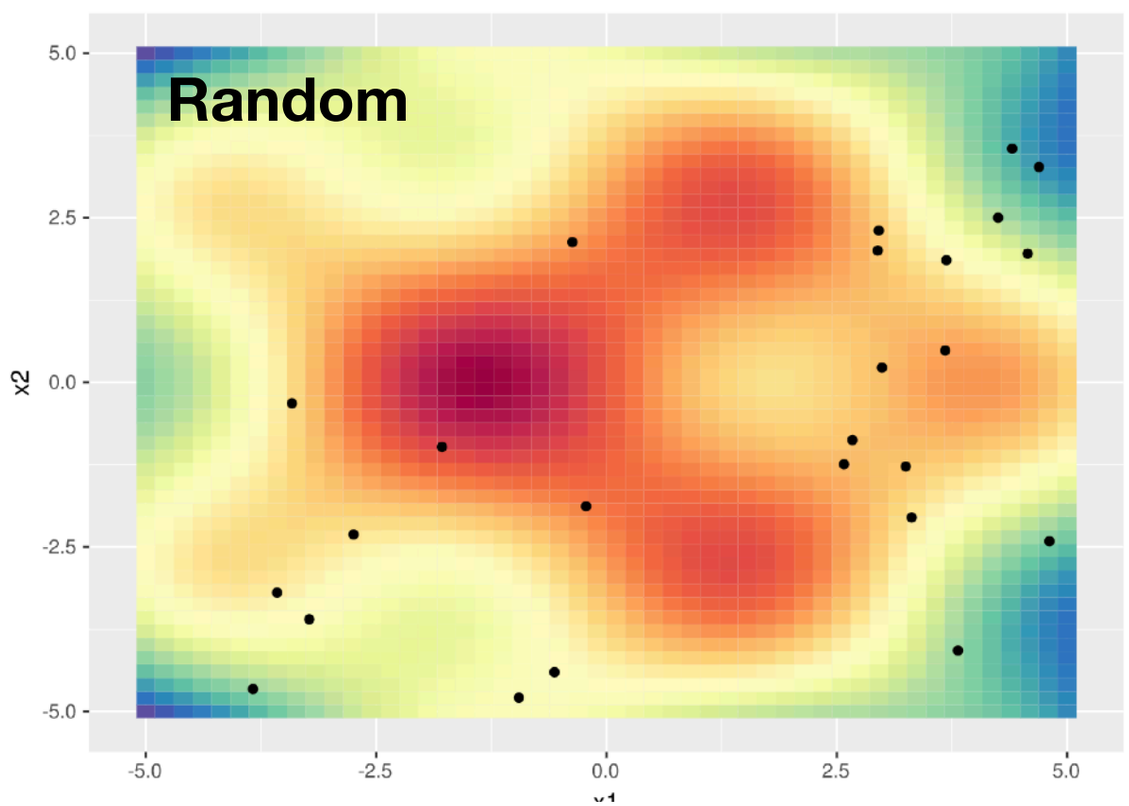
- Also works for non-convex, noisy data

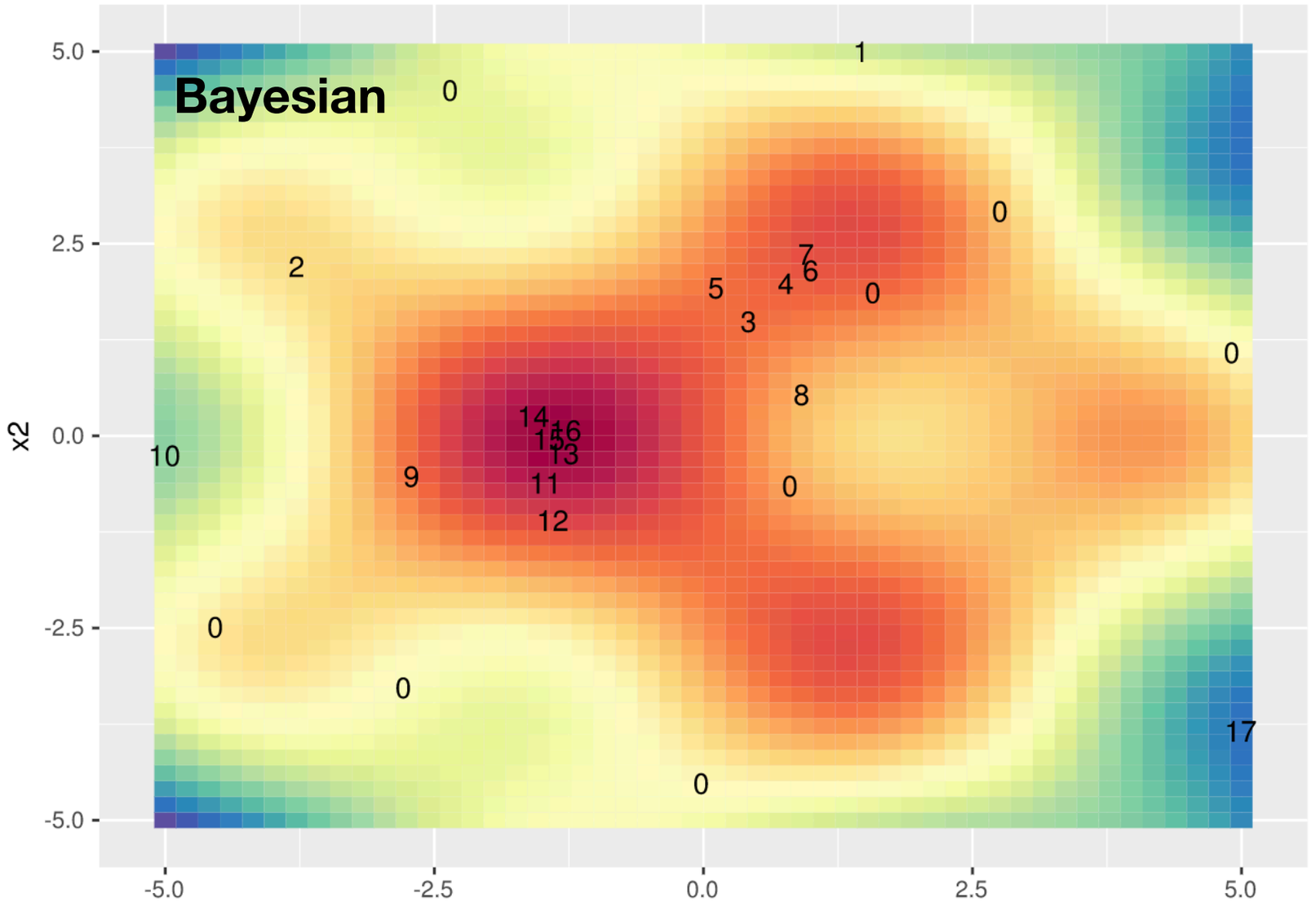







Grid
5.0
2.5
0.0
-2.5
-5.0
x2
-5.0
-2.5
0.0
2.5
5.0


Random
5.0
2.5
0.0
-2.5
-5.0
x2
-5.0
-2.5
0.0
2.5
5.0


Bayesian
5.0
2.5
0.0
-2.5
-5.0
x2
-5.0
-2.5
0.0
2.5
5.0
1
0
2
0
7
6
5
4
0
3
0
8
14
16
15
13
10
9
11
0
12
0
0
17
0

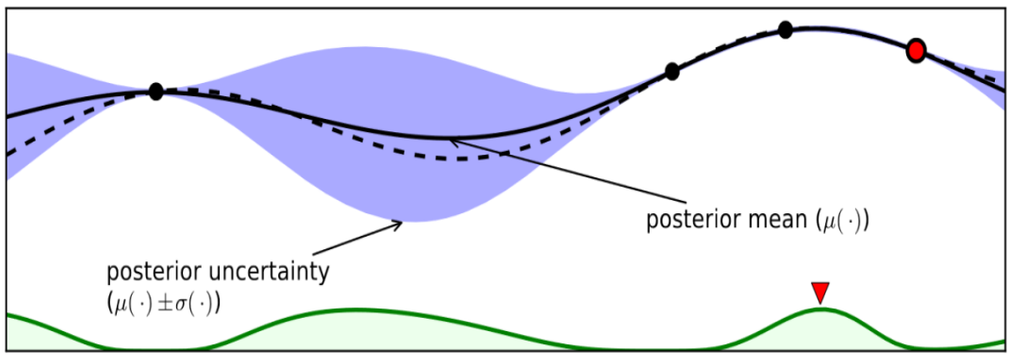
Bayesian Optimization: which surrogate?

Gaussian processes *[skopt]*

+ handles uncertainty, extrapolates well

+ ideal for few numeric hyperparameters

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

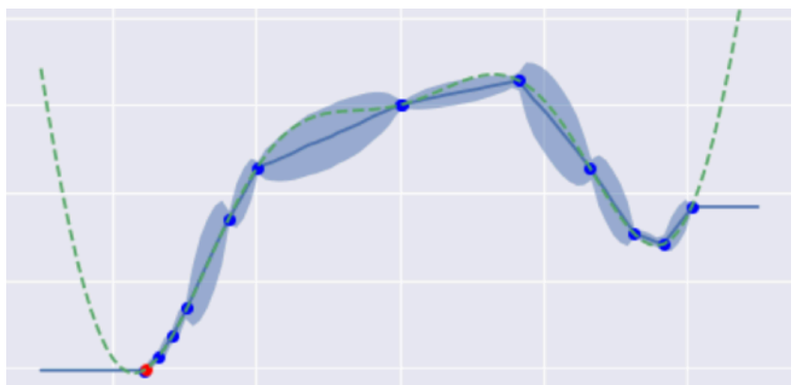


Random Forests *[Hutter et al. 2011, Feurer et al. 2015]* *[SMAC, auto-sklearn]*

Uses variance in individual tree predictions as uncertainty estimate

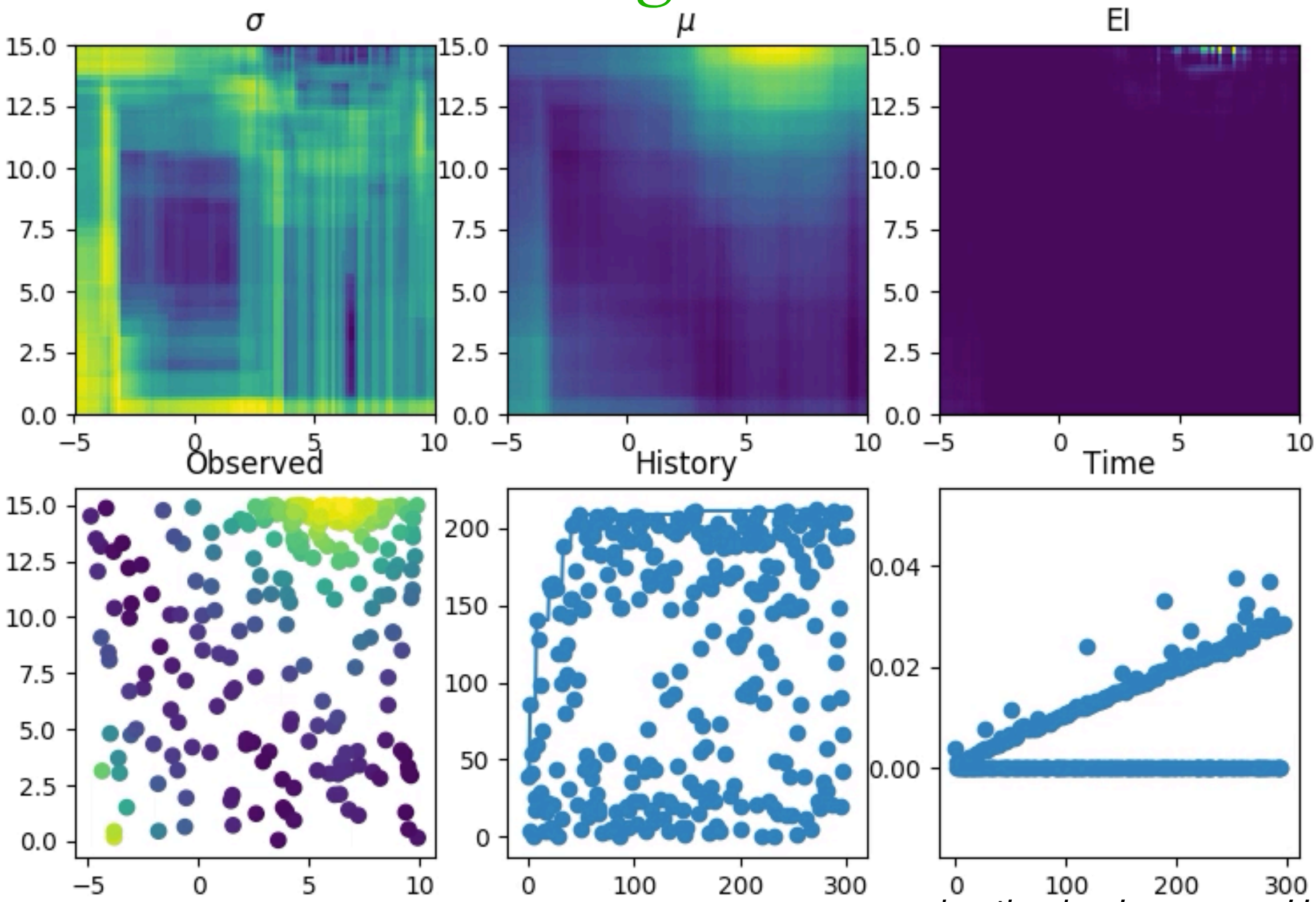
+ scalable, handles conditional hyperparams

- bad uncertainty estimates, extrapolation



```
>>> import autosklearn.classification
>>> cls = autosklearn.classification.AutoSklearnClassifier()
>>> cls.fit(X_train, y_train)
>>> predictions = cls.predict(X_test)
```

Random Forest Surrogate



animation by Jeroen van Hoof

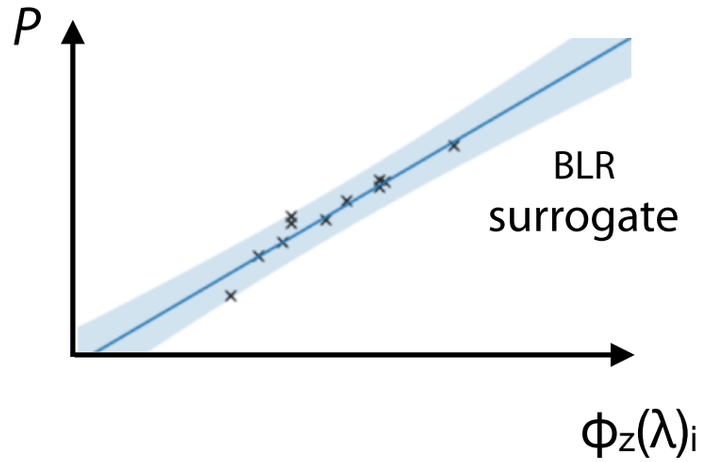
Bayesian Optimization: which surrogate?

Bayesian Linear Regression [Snoek et al. 2015] [Perrone et al. 2018] (Amazon AutoML)

Learn a basis expansion for the hyperparameter space, so that they can be modelled with (Bayesian) linear regression (linear complexity)

\+ Scalable, Bayesian

\- requires good basis expansion



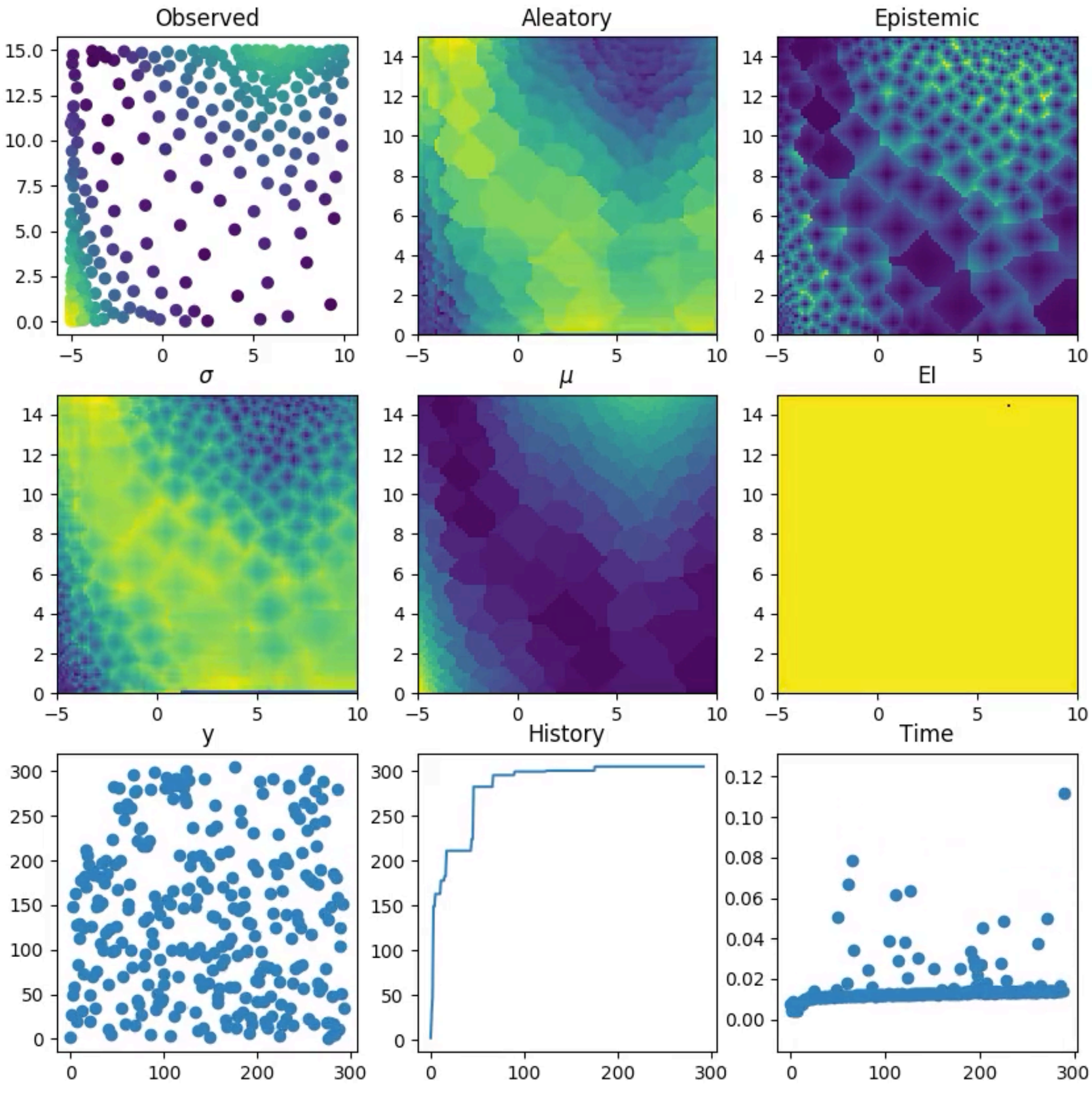
Hyperboost: Boosting + quantile regression [van Hoof, Vanschoren 2019]

Acquisition function based on predicted performance ($q_{0.9}$) based on LightGBM surrogate and distance to nearest observation

\+ better fit than RF, handles conditionals, adapts to drift

\- new, experimental

Gradient Boosting Surrogate



Hyperparameter optimization

[Komer et al. 2019]

Tree of Parzen Estimators

1.Test some hyperparameters

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

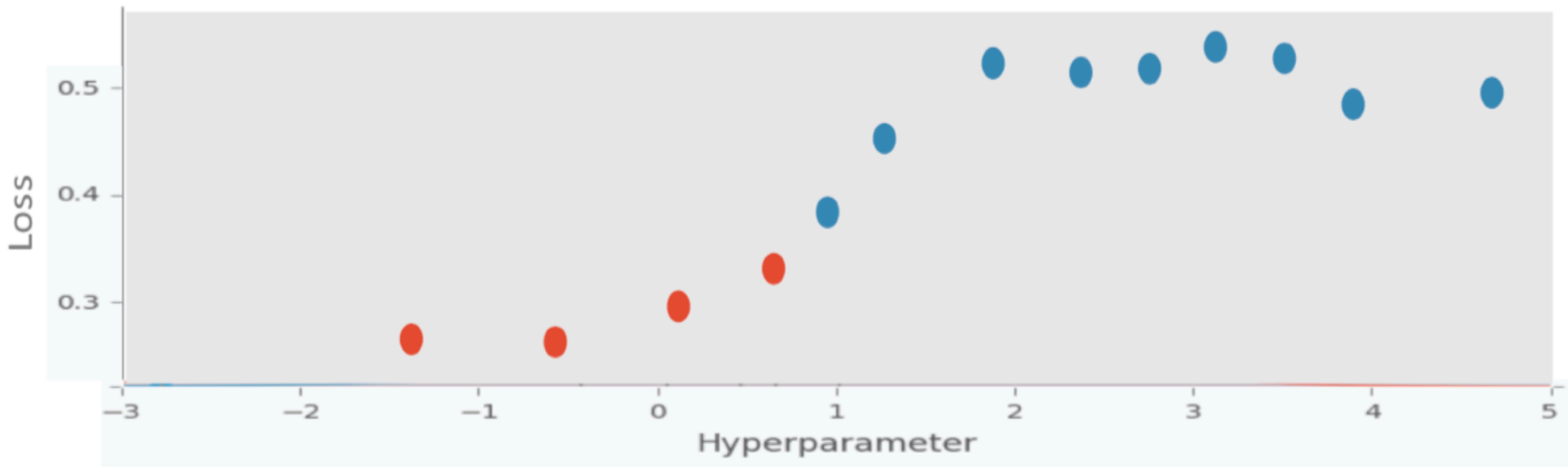
3. Fit non-parametric KDE for $p(\lambda = \text{good})$ and $p(\lambda = \text{bad})$

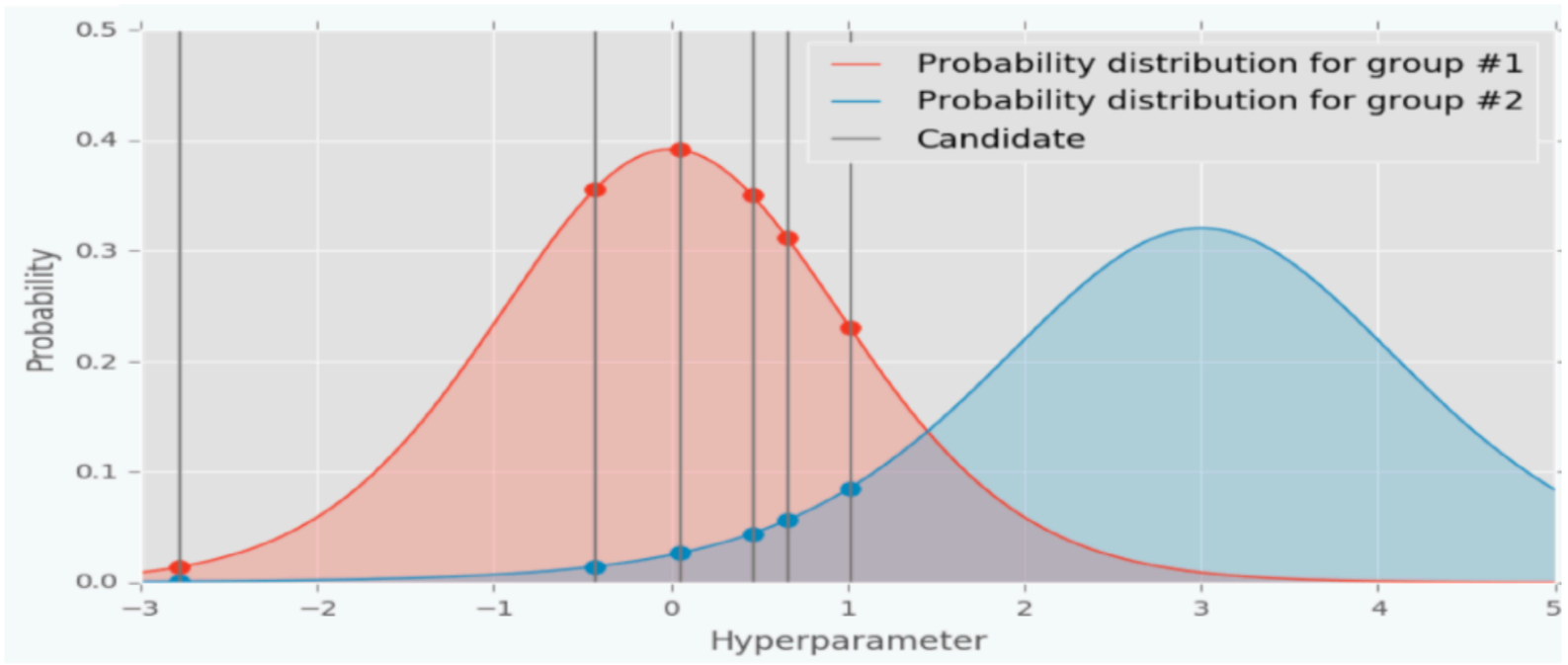
4. For a few samples, evaluate

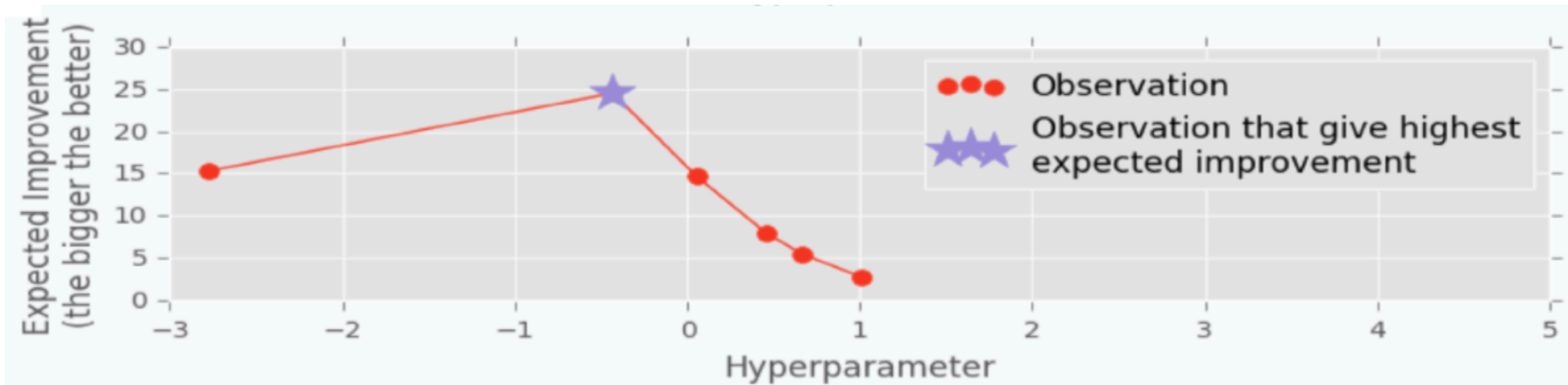
$$\frac{p(\lambda = \text{good})}{p(\lambda = \text{bad})}$$

Shown to be equivalent to EI!

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





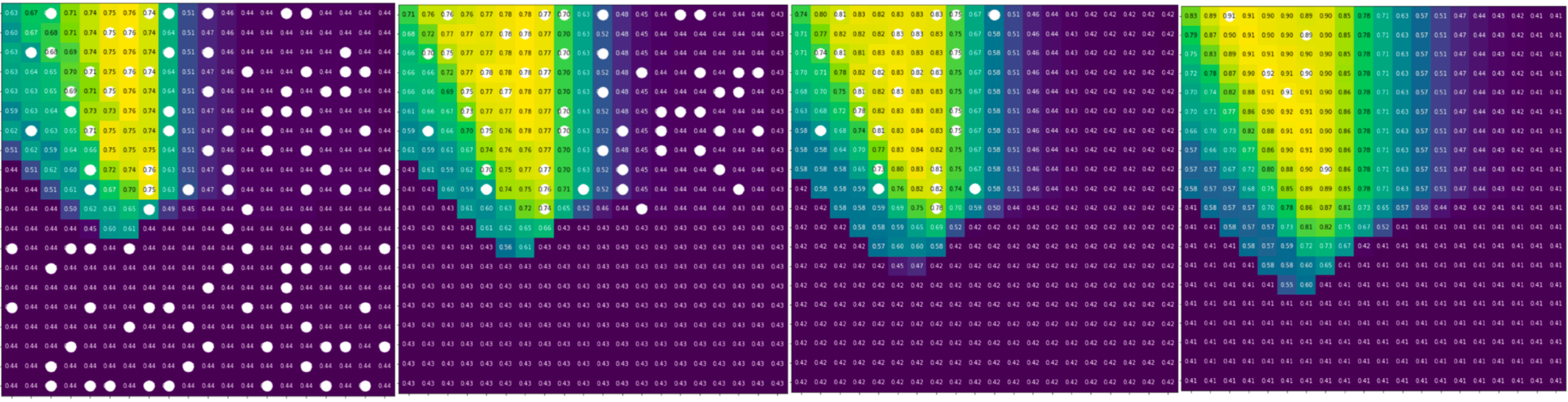


Jamieson & Talwalkar 2016

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



1/16 1/8 1/4 1/2

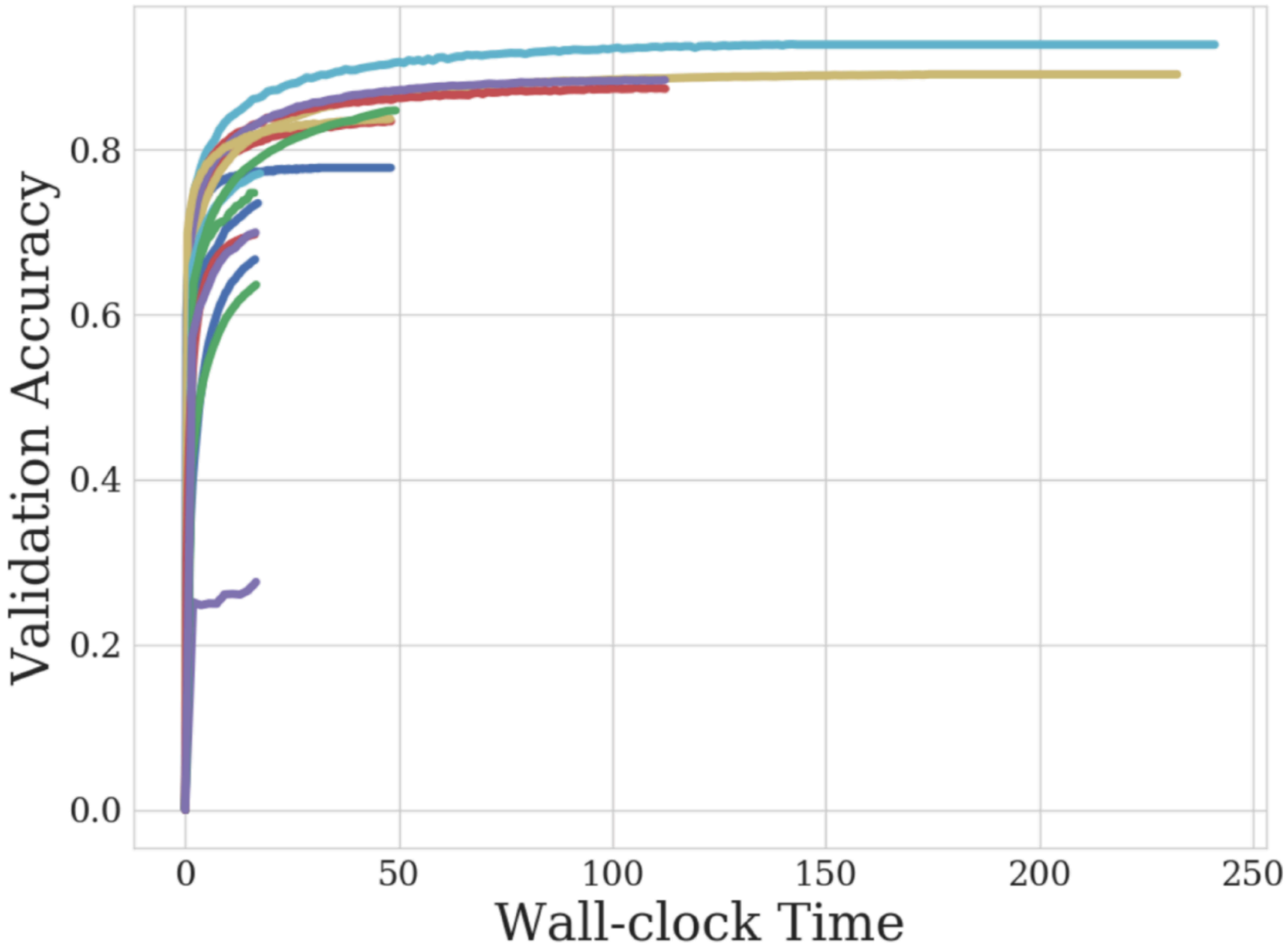
sample size

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

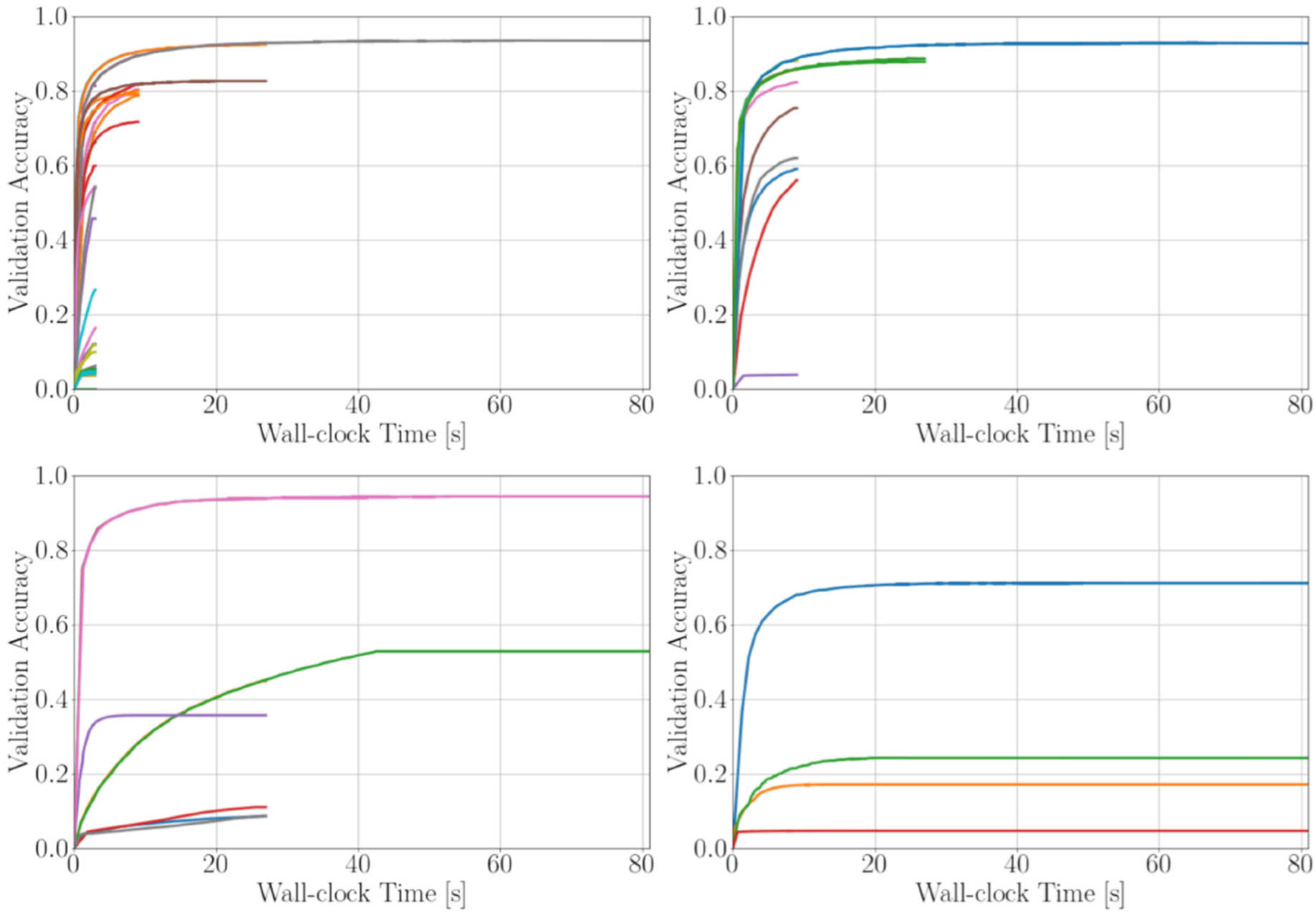


Li et al. 2017

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



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

Implementations exist for Keras / TensorFlow

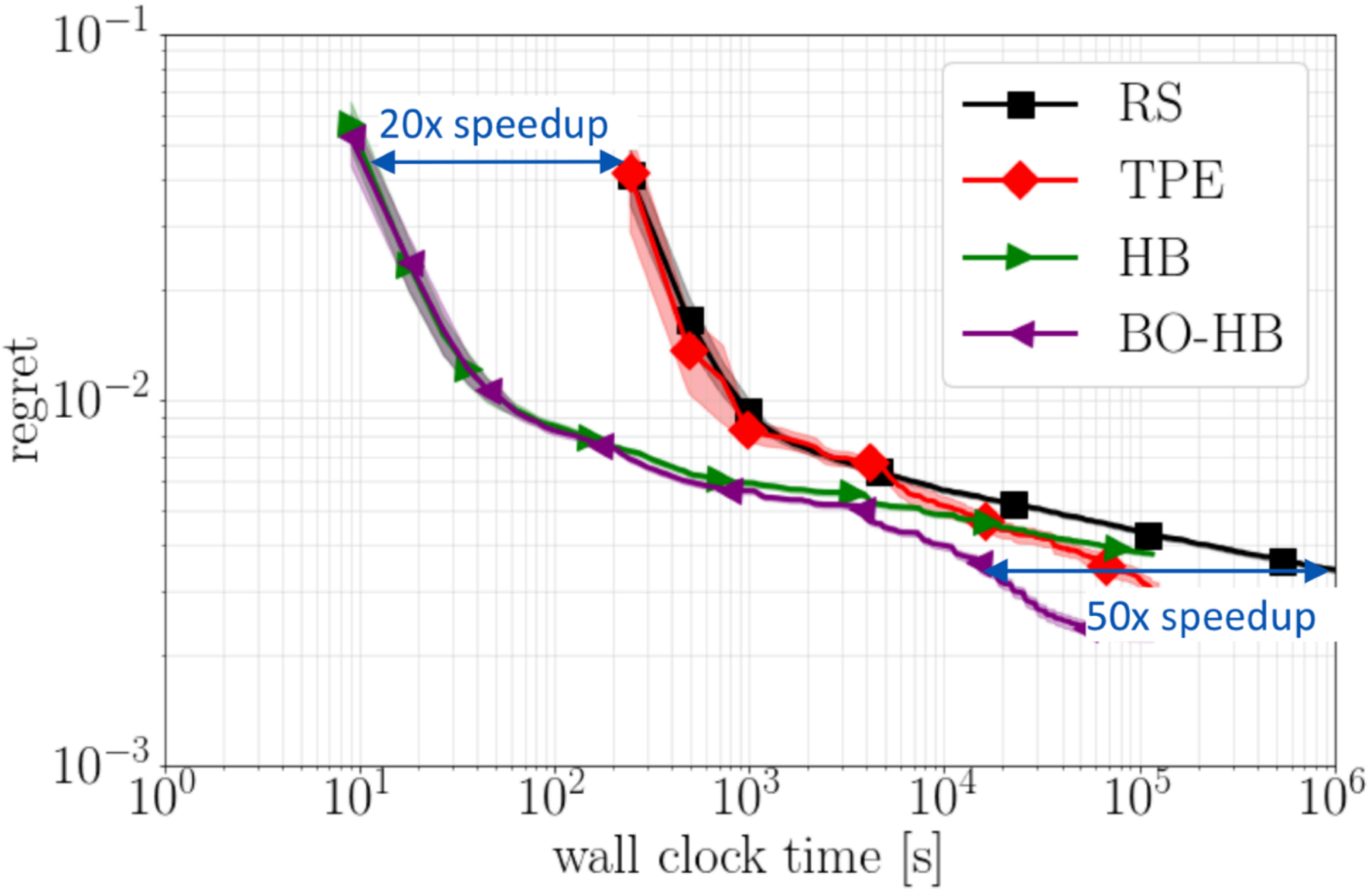
```
from kerastuner.tuners import Hyperband

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

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



Bayesian Optimization for NAS

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

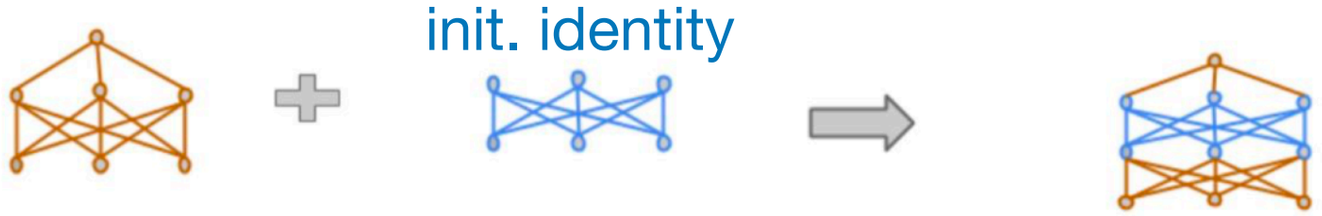
- AutoPyTorch[1] : DNNs+CNNs, 63 hyperparameters, tuned with BO-HB
- Joint NAS + HPO[2]: ResNets, tuned with BO-HB
- PNAS (Progressive NAS)[3]
  - Cell search space, optimized with SMAC, HPO afterwards
  - SotA on ImageNet, CIFAR

```
# running Auto-PyTorch
autoPyTorch = AutoNetClassification("tiny_cs",  # config preset
                                    log_level='info',
                                    max_runtime=300,
                                    min_budget=30,
                                    max_budget=90)

autoPyTorch.fit(X_train, y_train, validation_split=0.3)
```

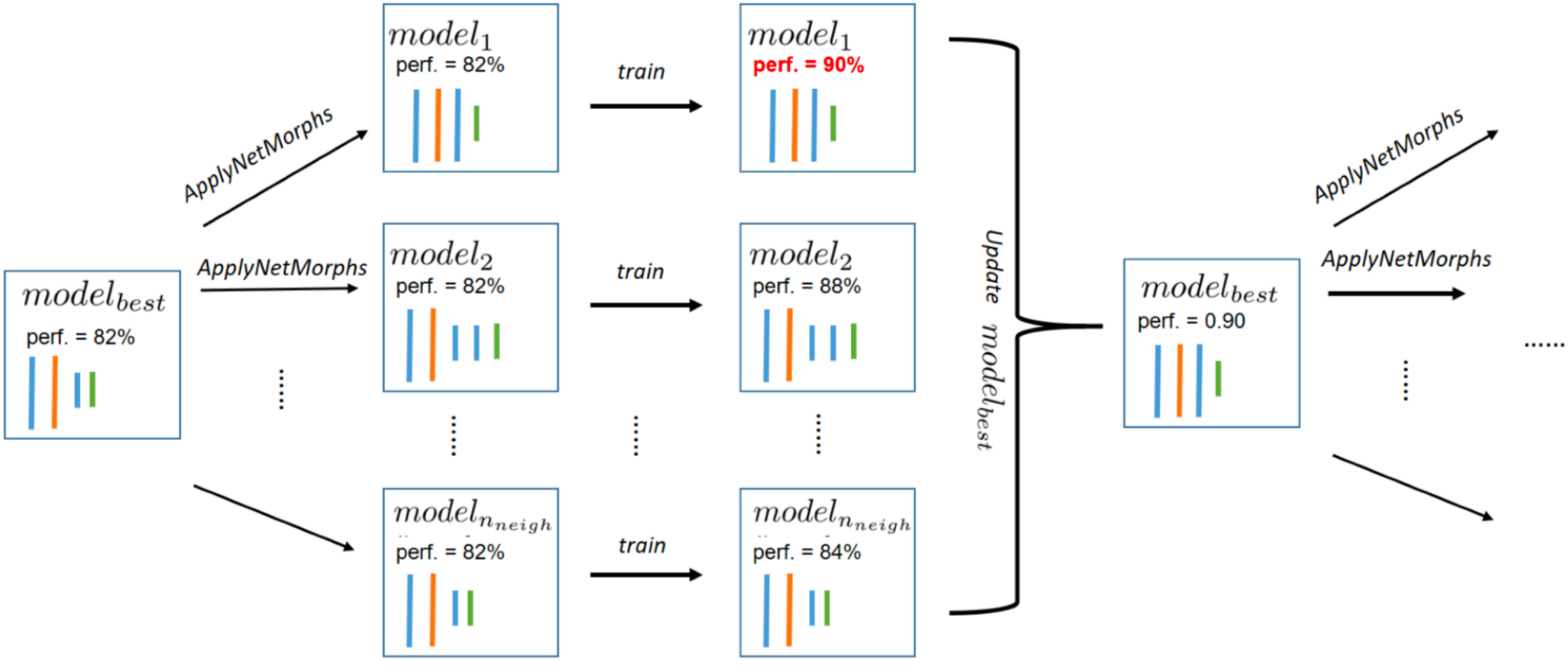
Chen et al. 2016, Wei et al. 2016, Cai et al. 2017
Cai et al. 2018, Elsken et al. 2017, Cortes et al. 2017, Cai et al. 2018

Network Morphisms

[AutoKeras]



- Speed up search
- Morphism: Changes architecture, but not modelled function
- Keep the initial weights, only update the derived architectures (faster)



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
- Keep the initial weights, only update the derived architectures
- AutoKeras: user defines high-level 'blocks', AutoML tunes them, guided by Bayesian optimization

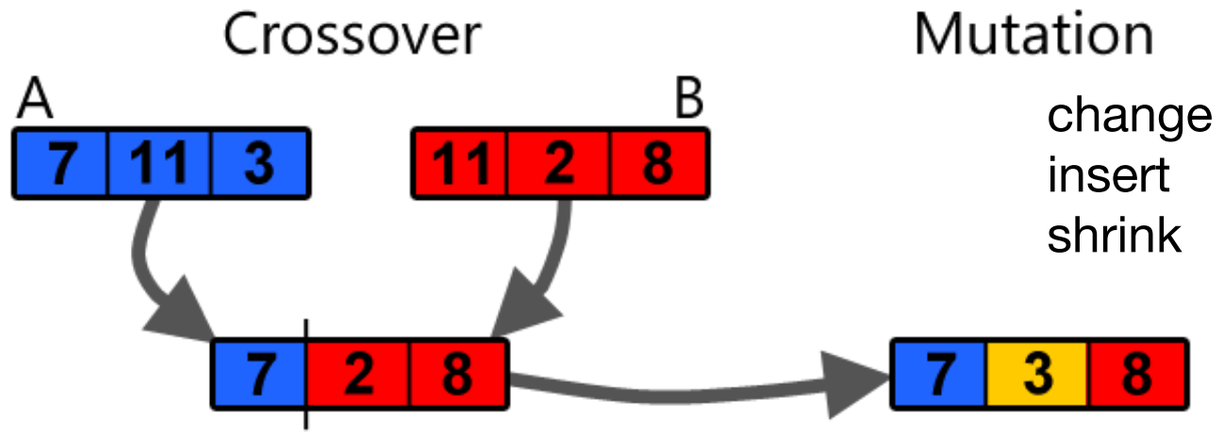
```
import autokeras as ak

# Initialize the image classifier.
clf = ak.ImageClassifier(max_trials=1) # It tries 10 different models.
# Feed the image classifier with training data.
clf.fit(x_train, y_train,epochs=3)
```

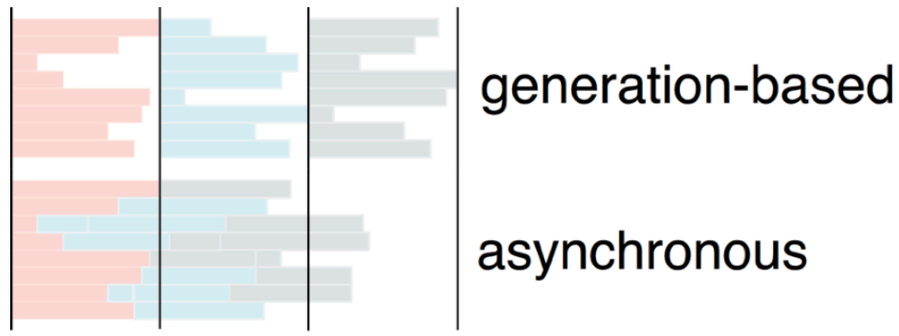
Evolution

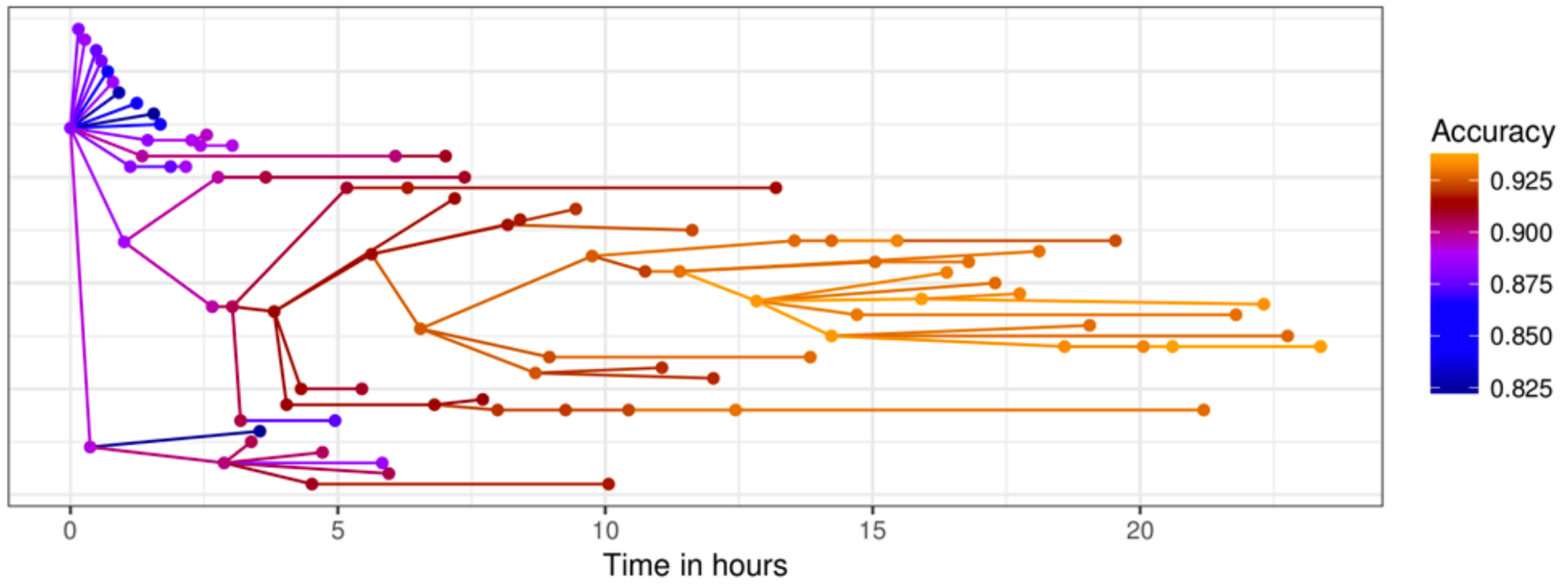
TPOT - *Olson & Moore 2016*

GAMA - *Gijsbers & Vanschoren 2018*

- Start with initial pipeline
- Best pipelines *evolve*: cross-over or mutation
  - Generation-based (TPOT)
  - Asynchronous (GAMA)
- Adapts pipeline to complexity of the problem
- Adapts quickly to evolving data



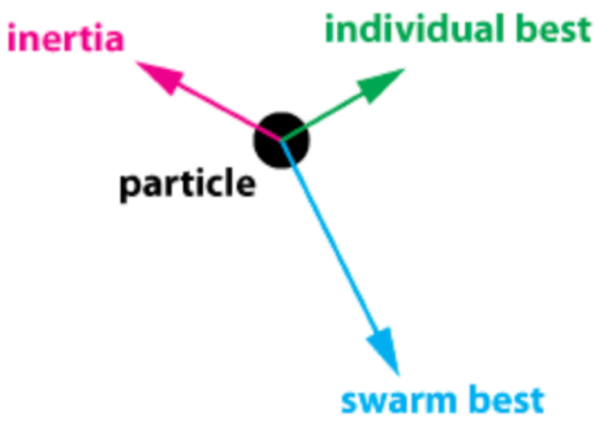


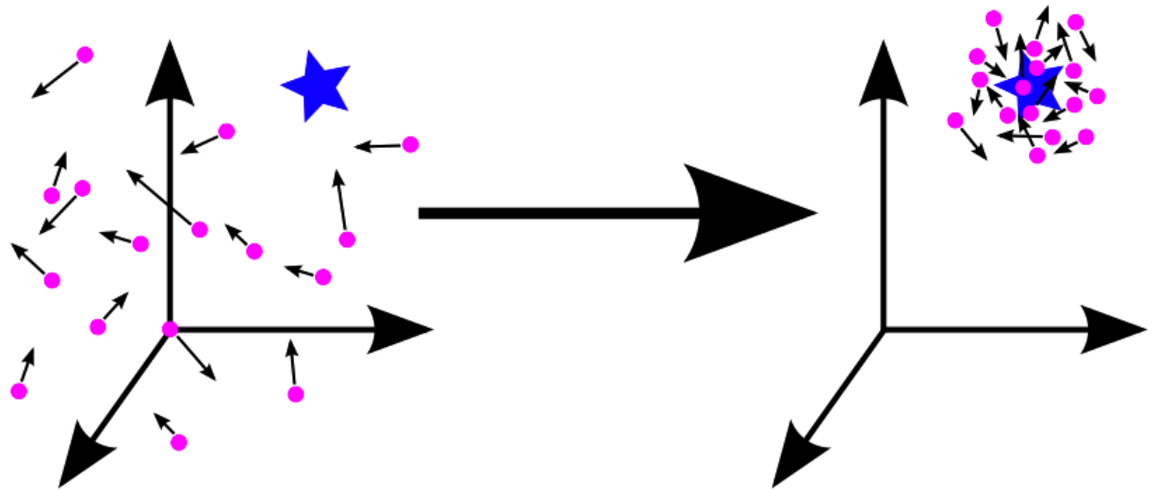


+ more flexible
- larger search space, can be slower

Evolution

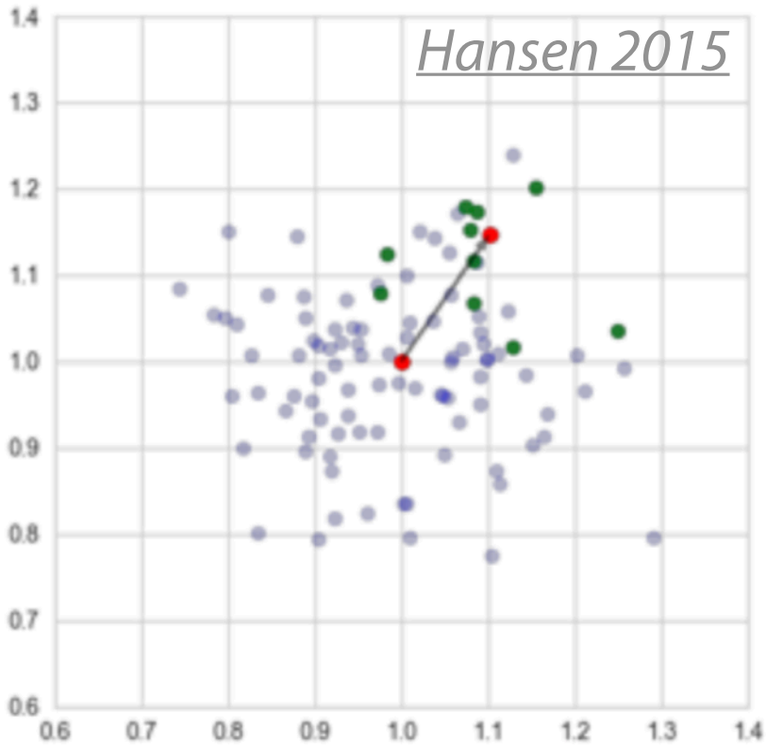
- Particle swarm optimization *[Mantovani et al 2015]*
  - Every configuration is a particle, influenced by other particles





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

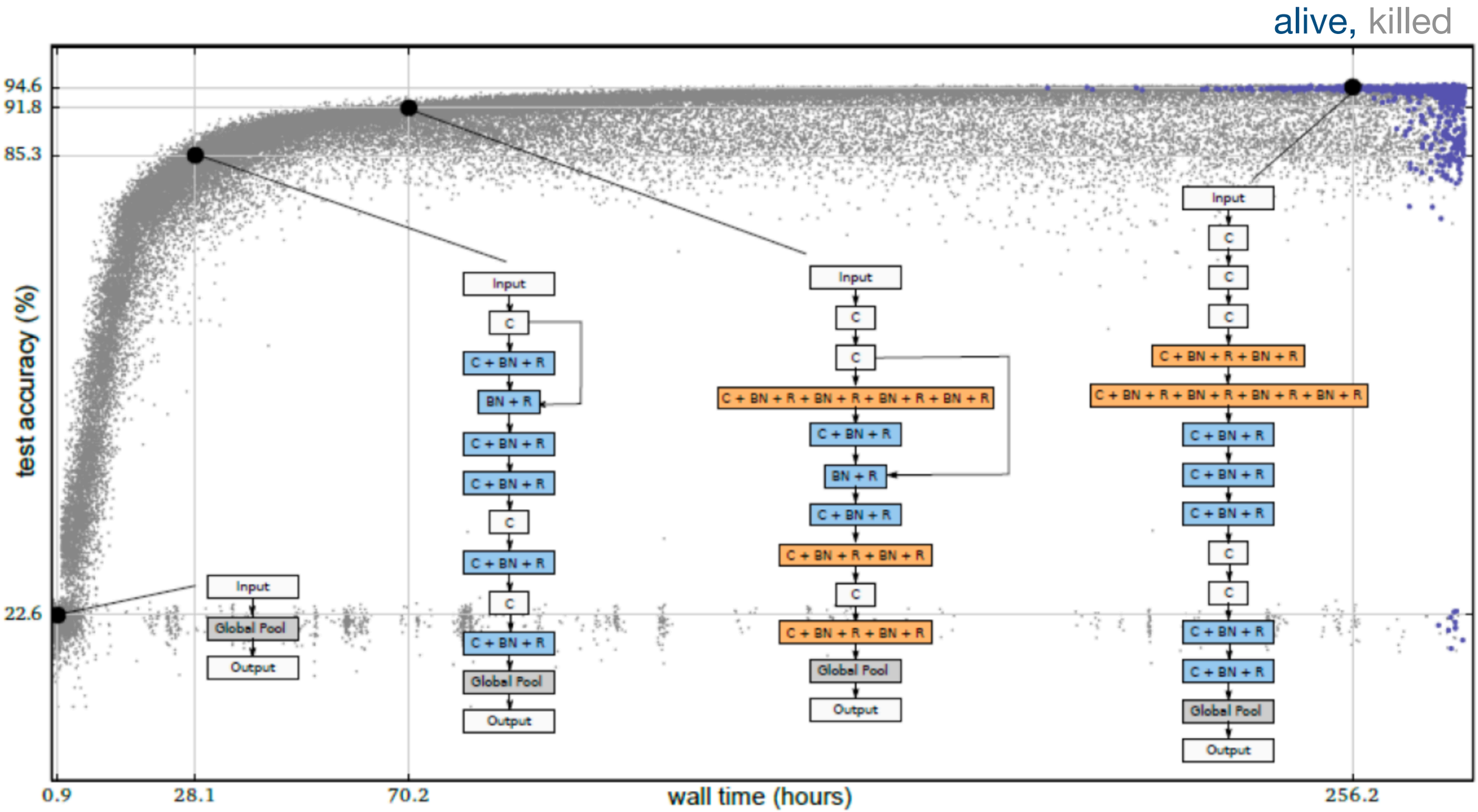
[Loshilov, Hutter 2016]



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

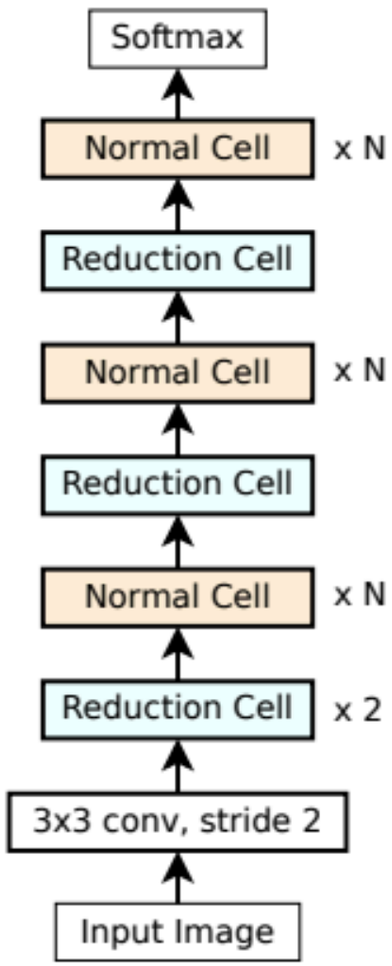


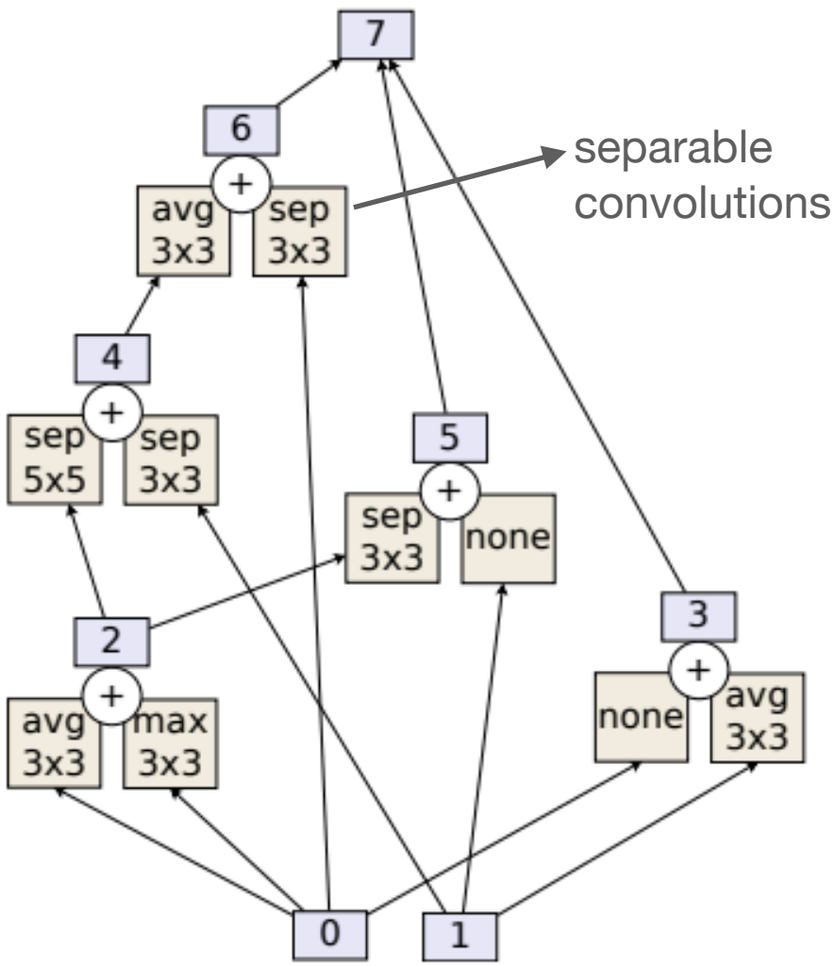
Real et al 2019

Neuro-evolution

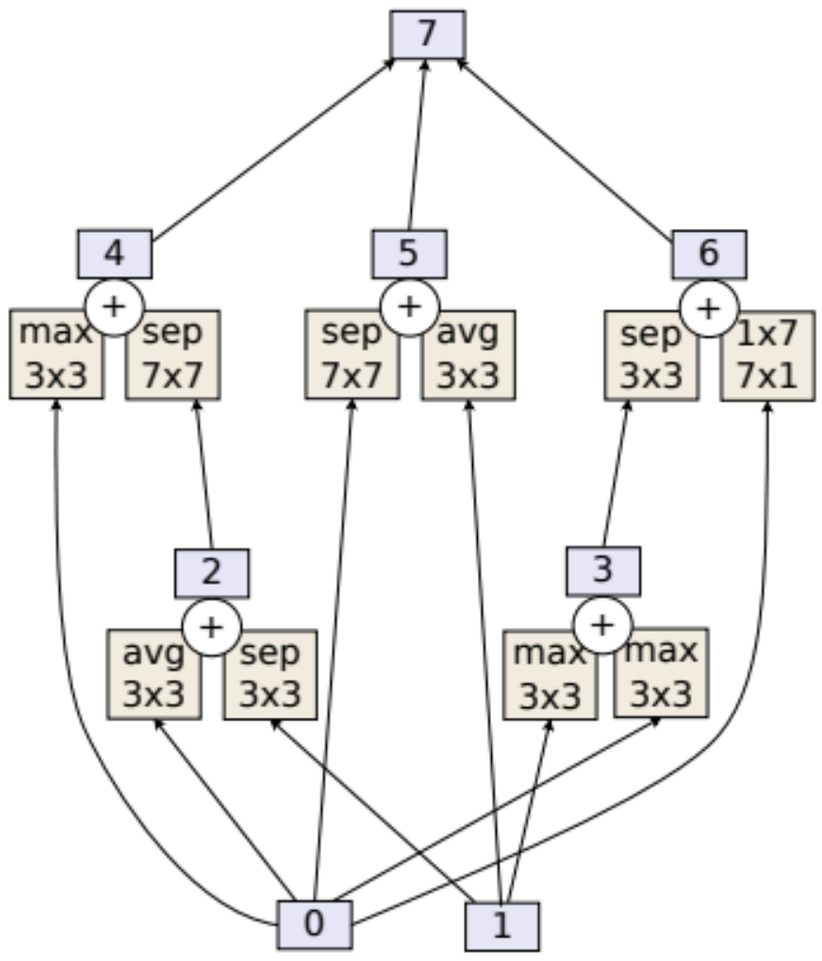
AmoebaNet: State of the art on ImageNet, CIFAR-10

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





normal cell



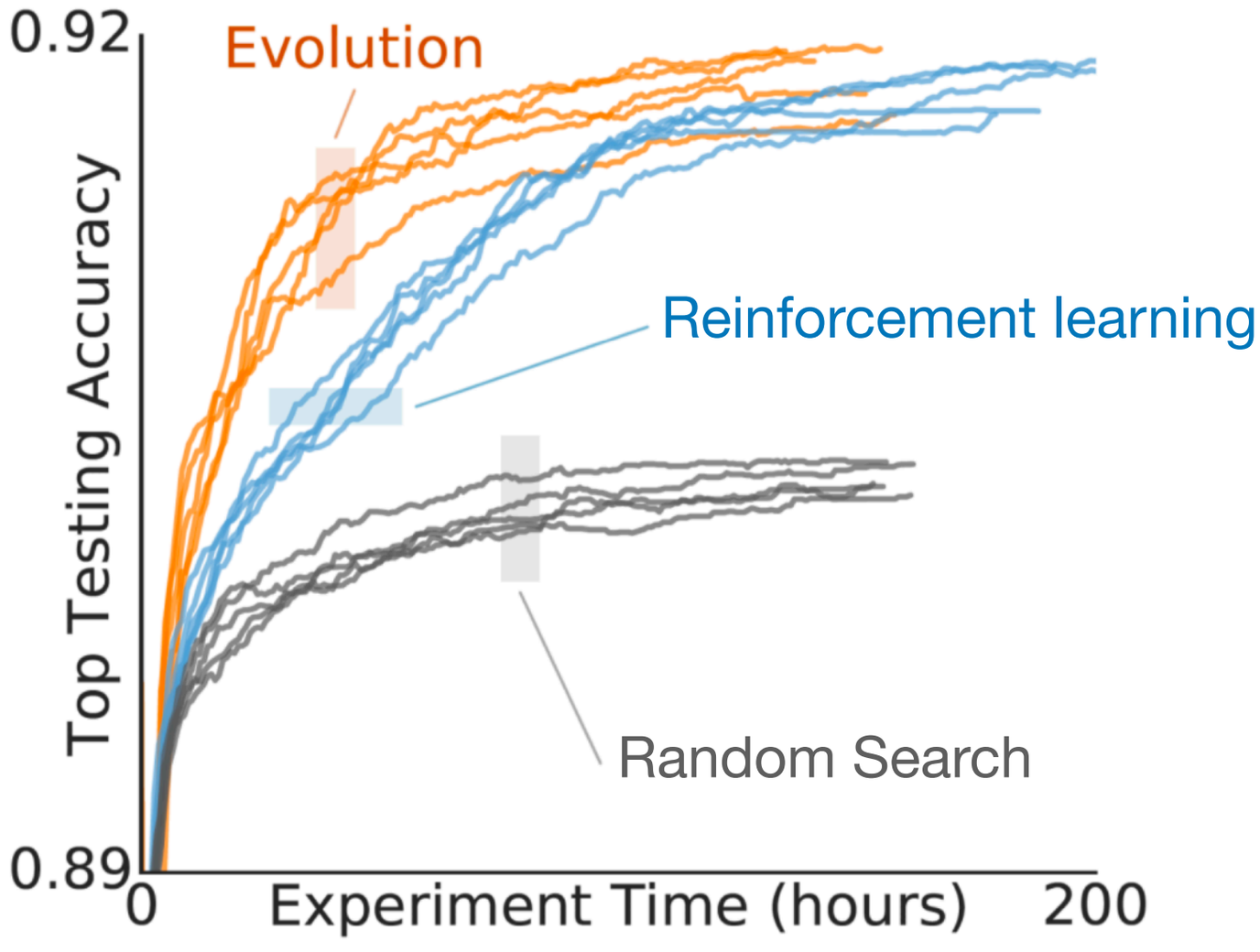
reduction cell

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

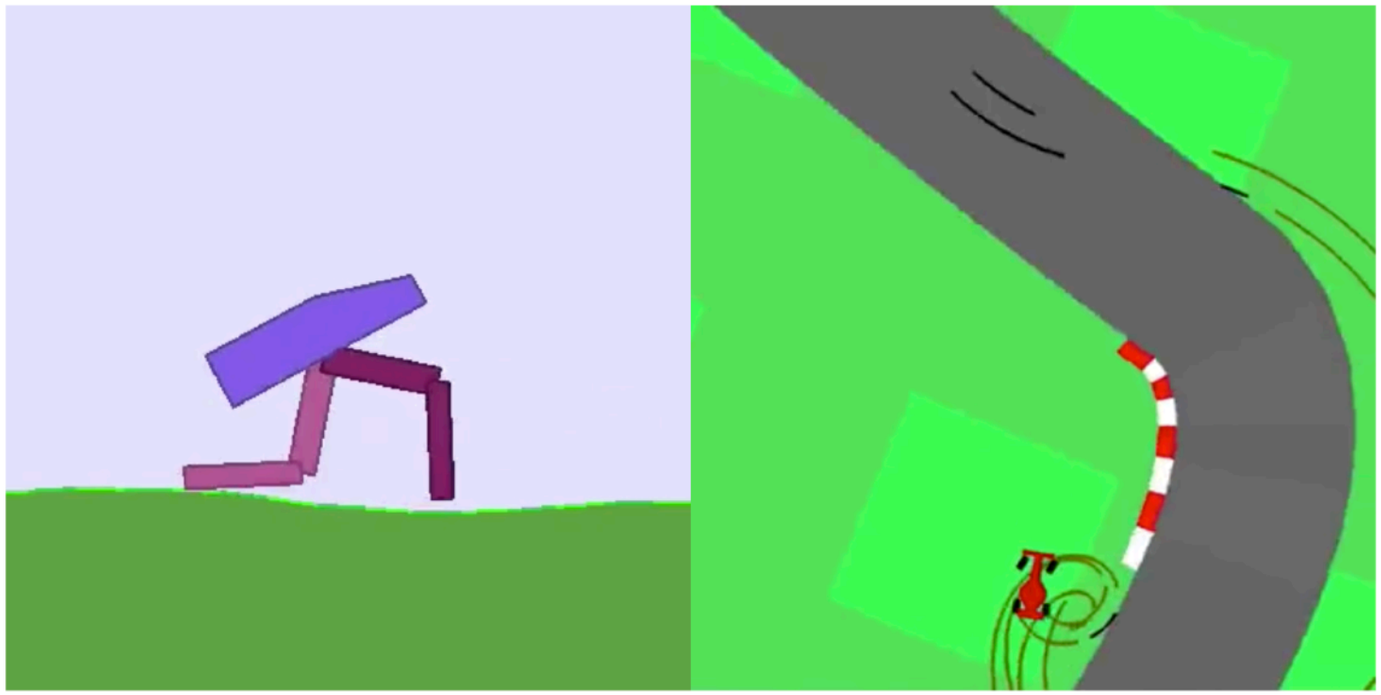


Gaier & Ha 2019

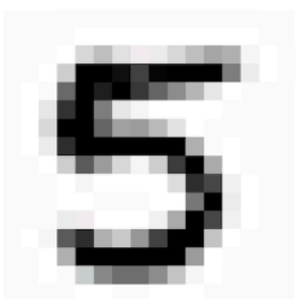
Weight-agnostic neural networks

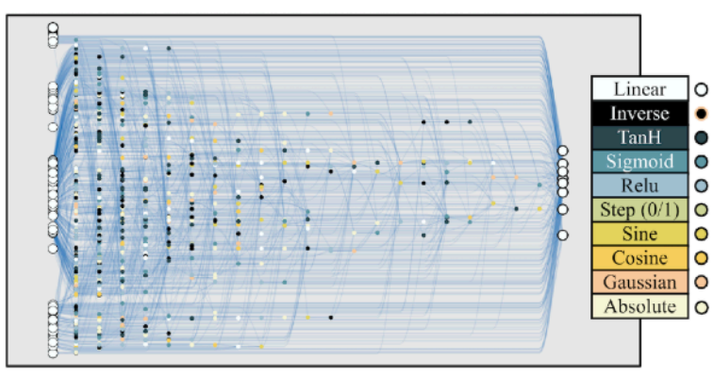
Evolving the networks while training the model weights is expensive

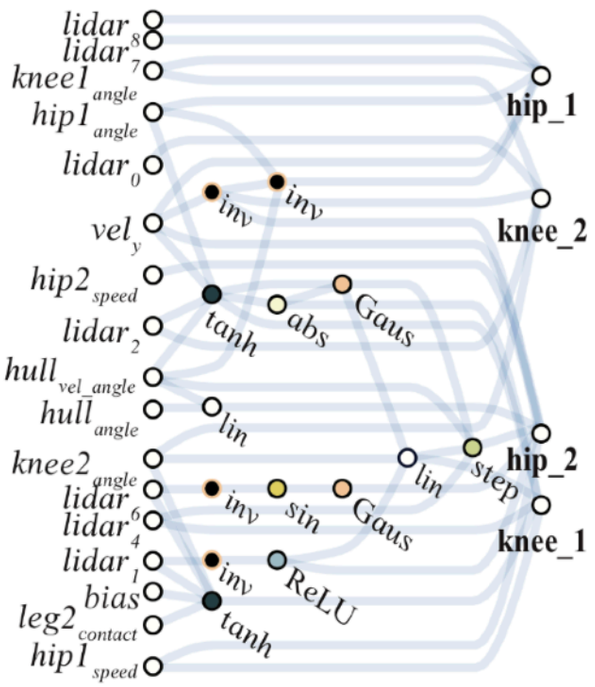
- Can we just fix the model weights and only evolve the architecture?

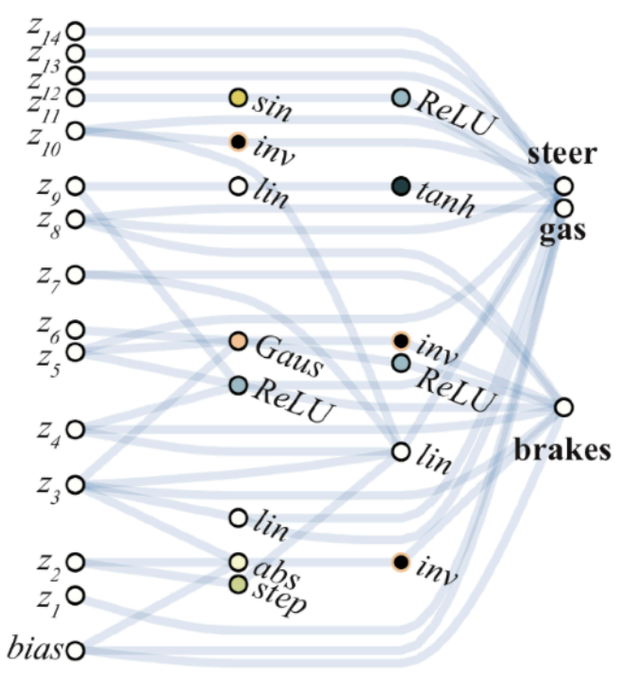


MNIST digit







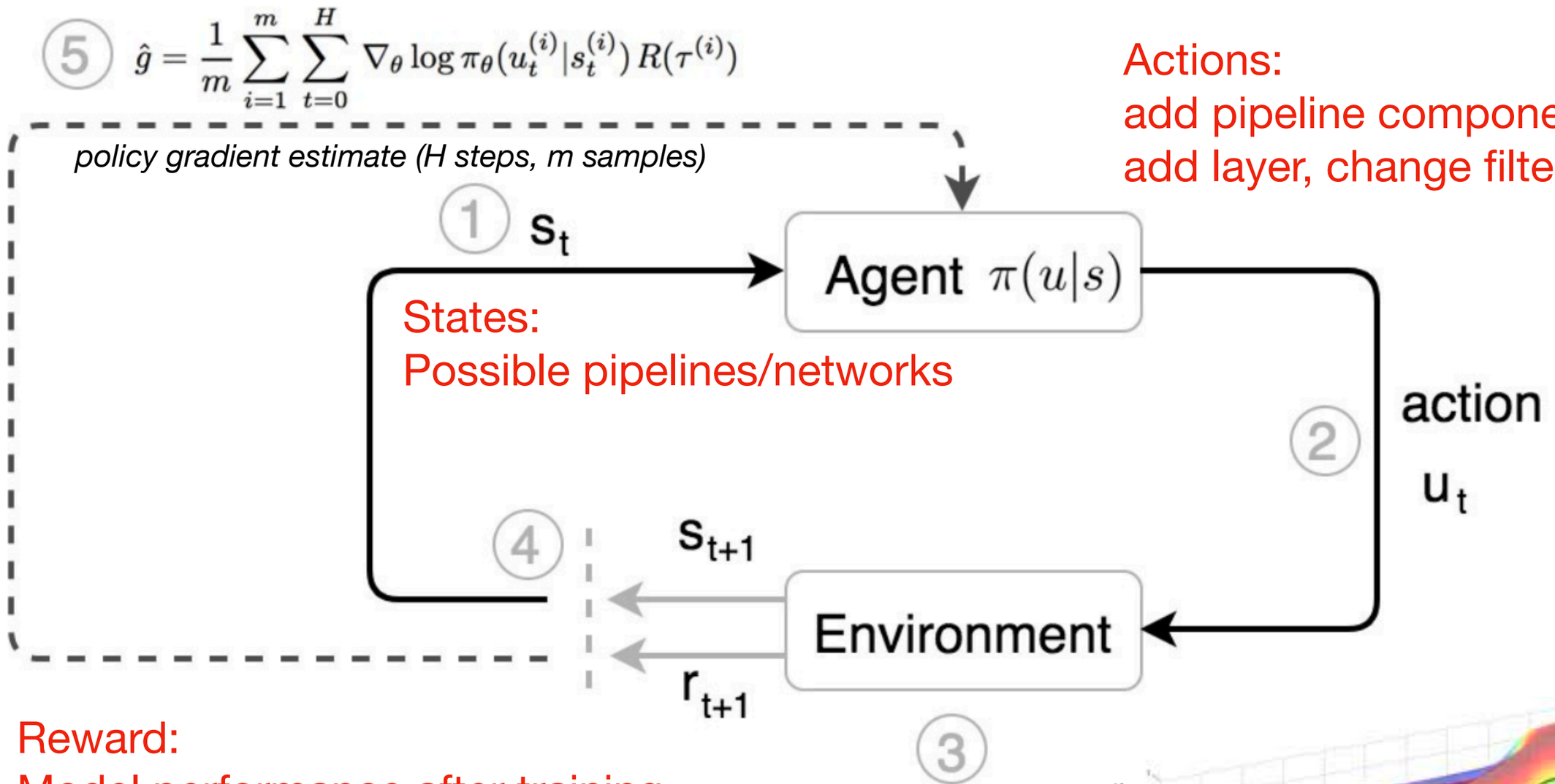


Zoph & Le 2017

Levine Hui

Reinforcement learning

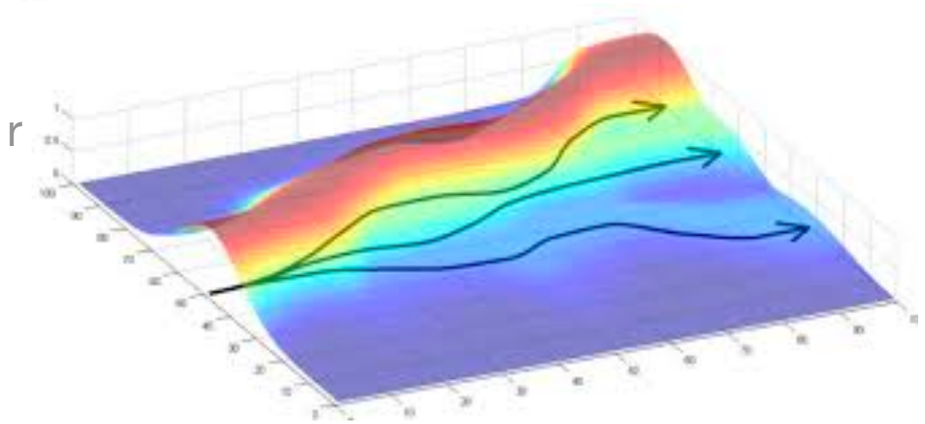
Build pipeline or network step-by-step, learn general strategy (policy)



Actions:
add pipeline component, tune,…
add layer, change filter size,…

Reward:
Model performance after training

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



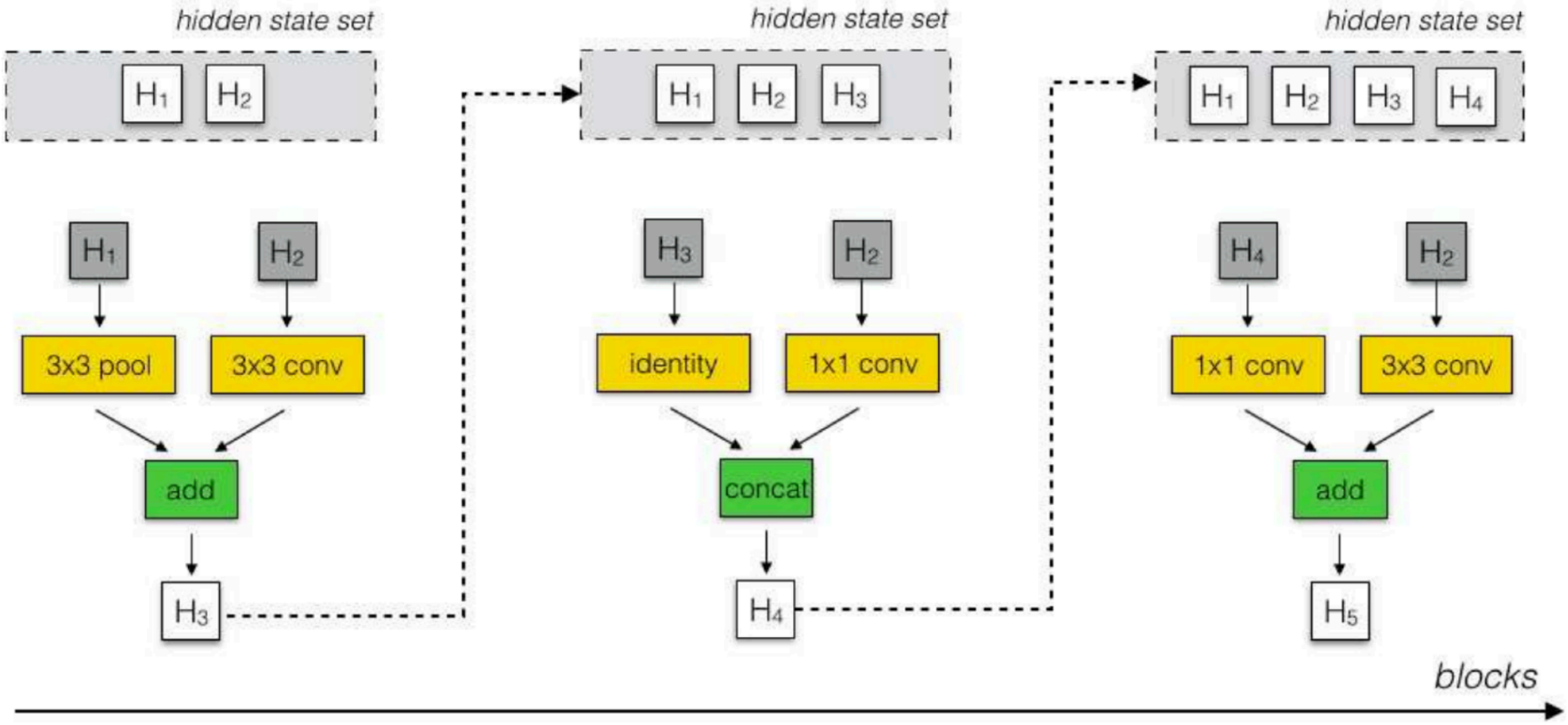
Zoph et al 2018
Zoph & Le 2017

NAS with Reinforcement learning

1-layer LSTM (PPO), cell space search

- State of the art on ImageNet
- 450 GPUs, 3-4 days, 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

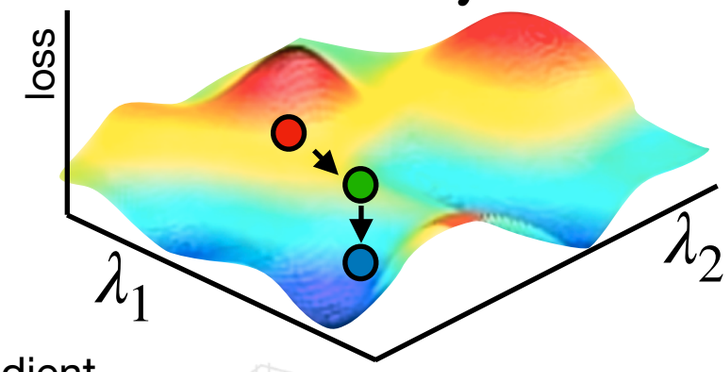


[MacLaurin et al 2015]
[Franceschi et al 2018]
[Luketina et al 2016]

Hyperparameter gradient descent

Optimize neural network hyperparameters λ and weights $\boldsymbol{w}$ simultaneously

- Compute *hypergradients* wrt. validation loss
  - Try multiple iterations with different λ
  - Compute gradient wrt loss to update λ



hypergradient

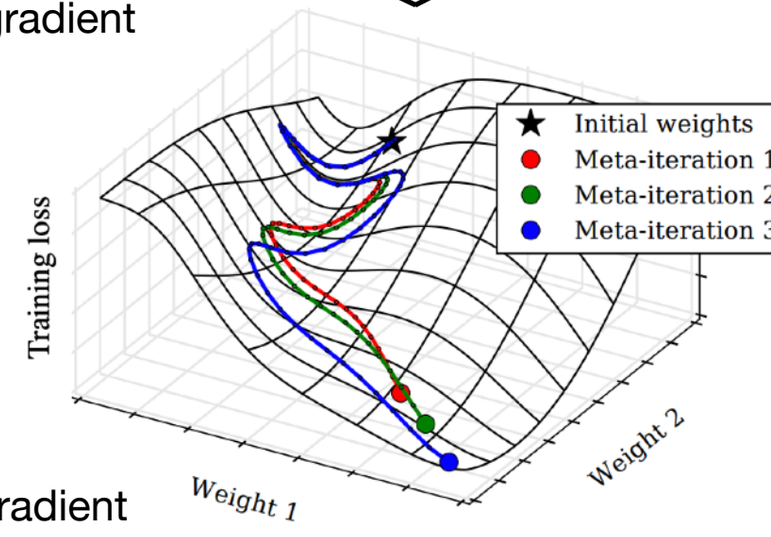
- Bilevel program
  - Outer obj.: optimize λ
  - Inner obj.: optimize weights given λ
    - Typically approximated

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

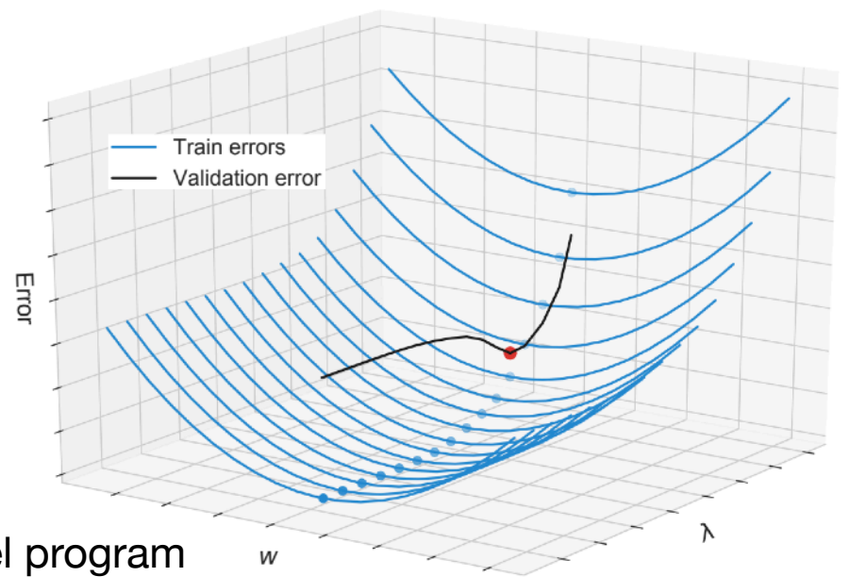
- Interleave optimization steps
  - Alternate SGD steps for ω and λ

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

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



weight gradient

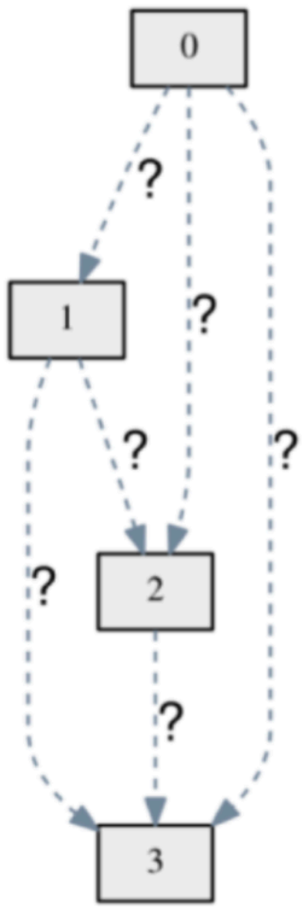


bilevel program

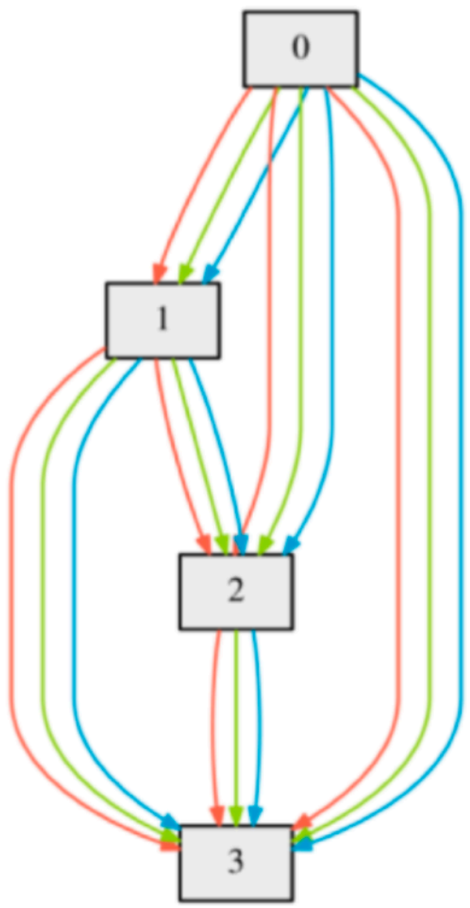
Liu et al. 2018

DARTS: Differentiable NAS

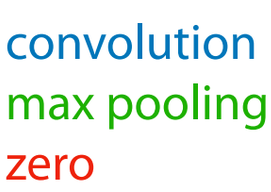
- Fixed (one-shot) structure, learn which operators to use
- Give all operators a weight α_i
- Optimize α_i and model weights ω_j using bilevel optimization
  - approximate $\omega_j^*(\alpha_i)$ by adapting ω_j after every training step

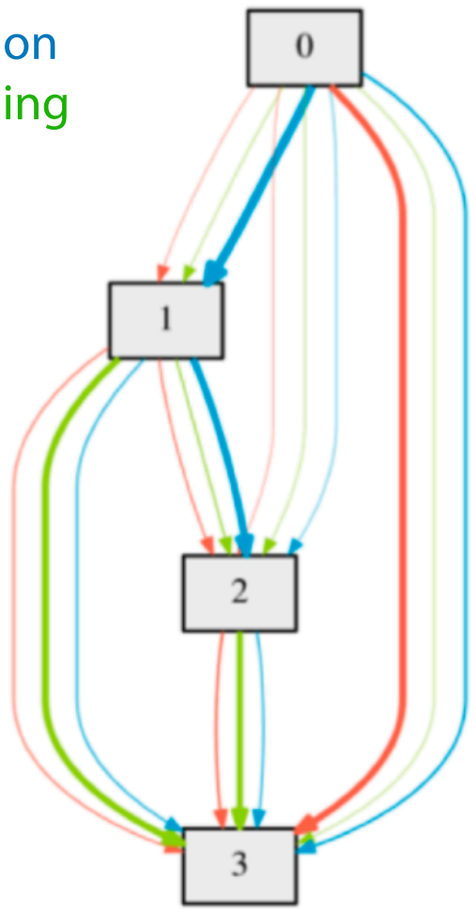


One-shot model

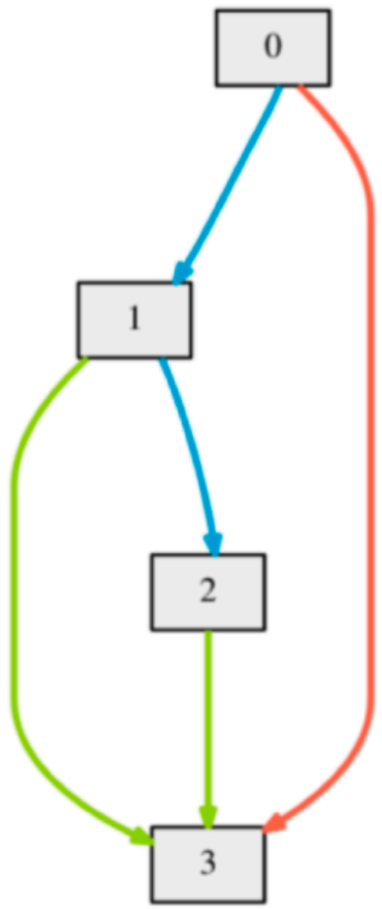


operator weights α_i





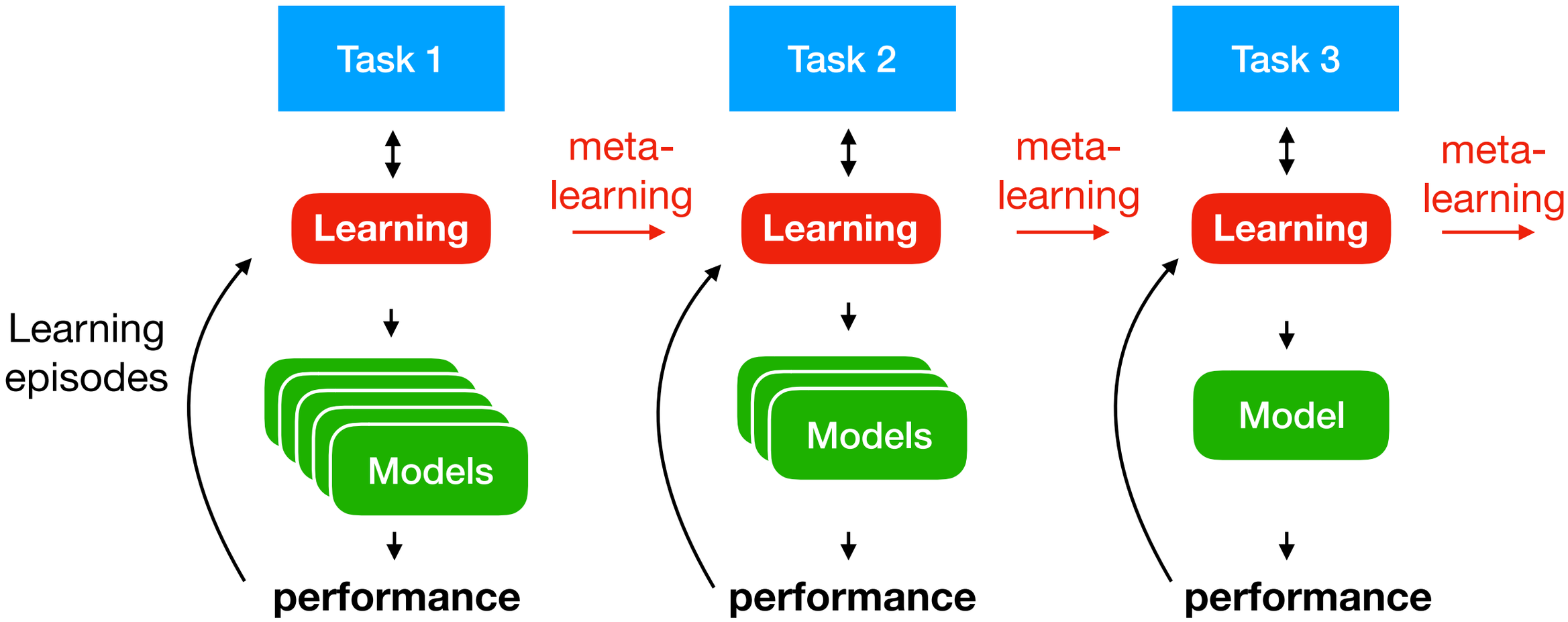
interleaved optimization of α_i and ω_j with SGD



argmax α_i

Learning is a never-ending process

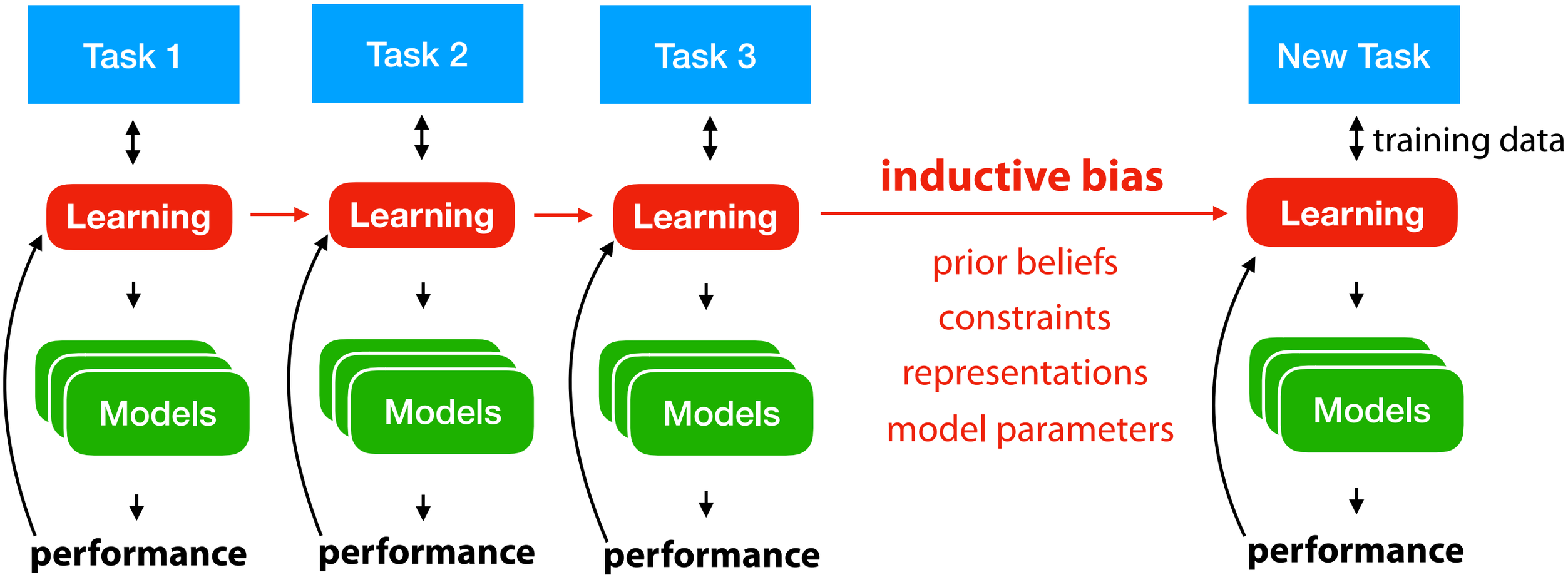
Humans learn *across* tasks
Why? Requires less trial-and-error, less data



Learning to learn

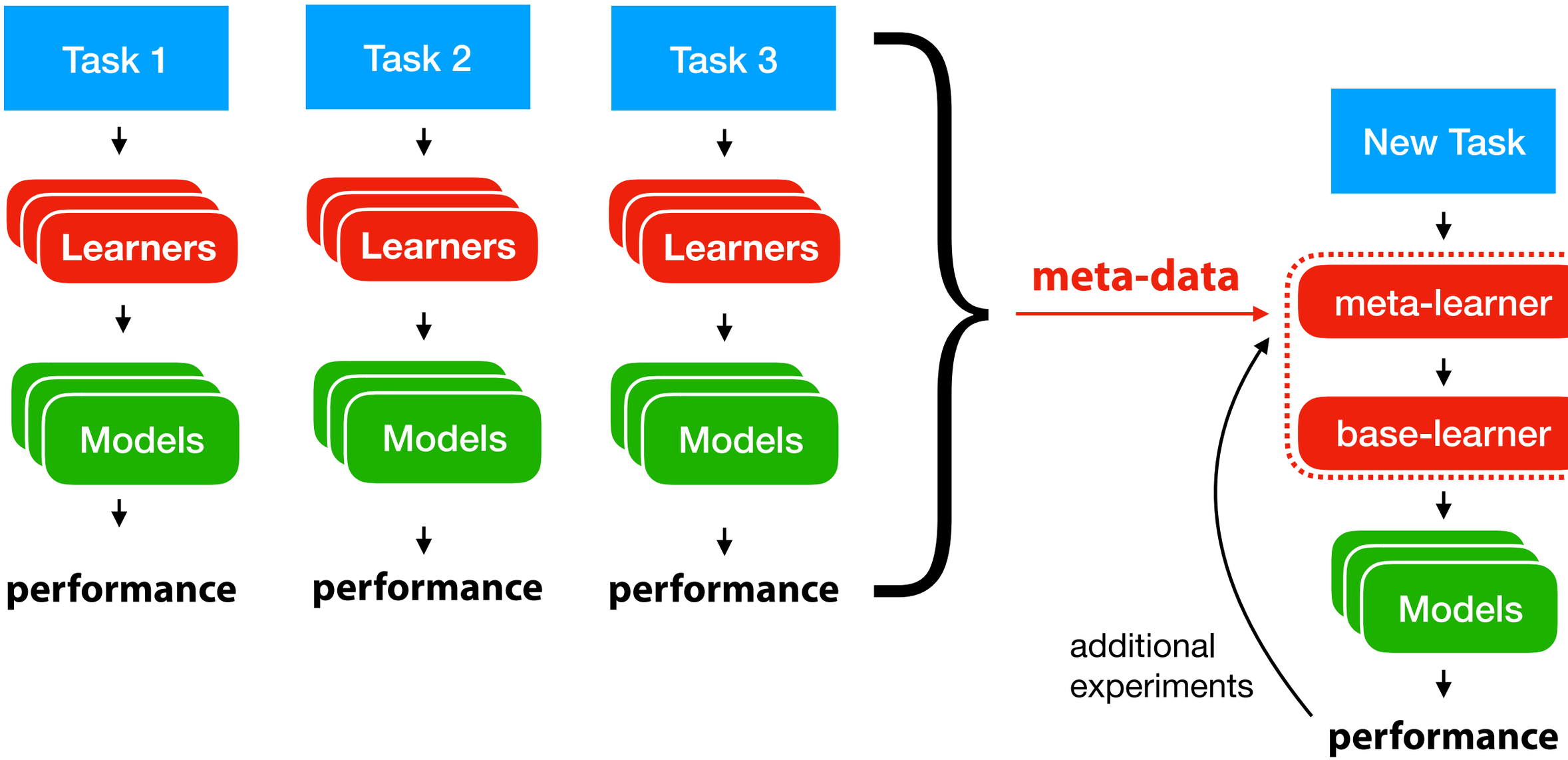
If prior tasks are *similar*, we can ***transfer*** prior knowledge to new tasks

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



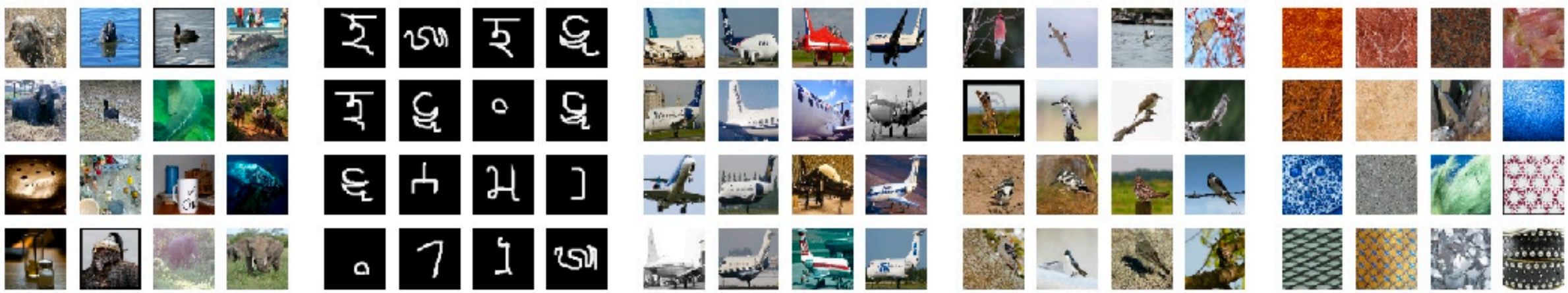
Meta-learning

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

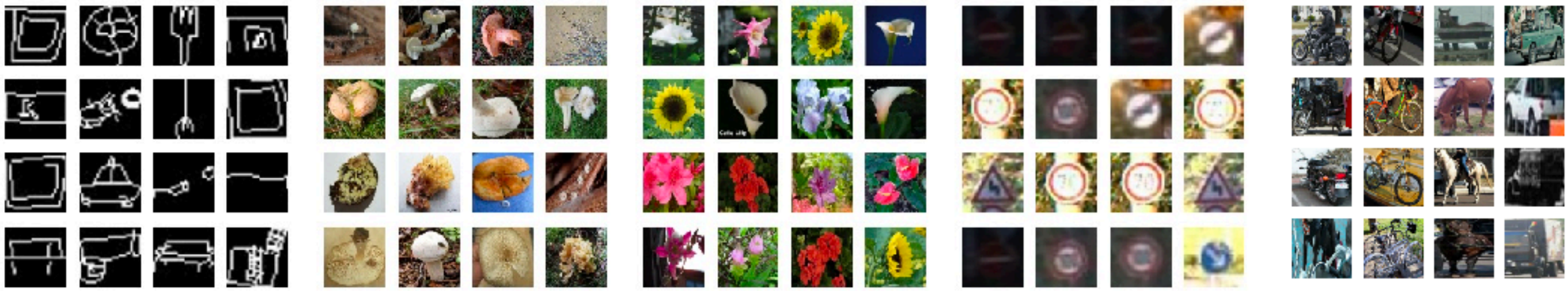


Triantafillou et al. 2019

Example: meta-dataset



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



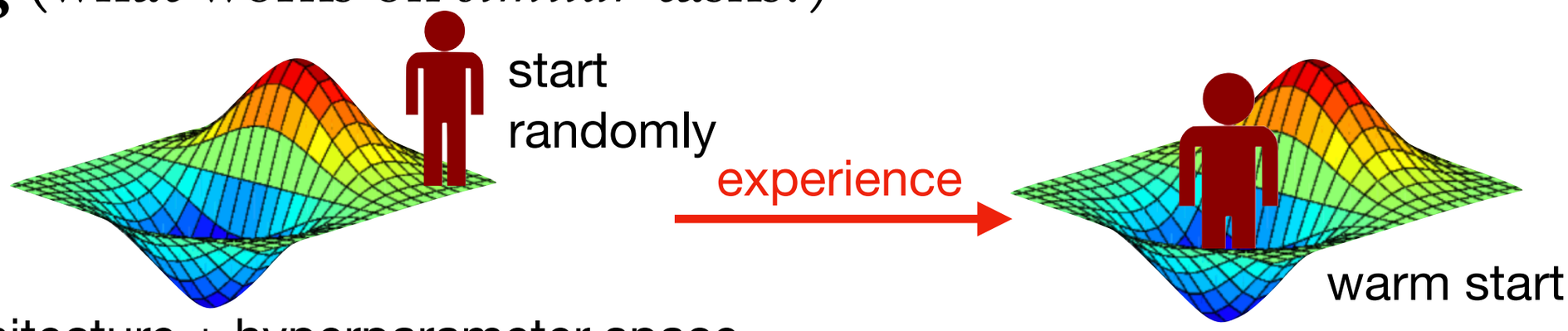
(f) Quick Draw (g) Fungi (h) VGG Flower (i) Traffic Signs (j) MSCOCO

How to learn how to learn?

Search space design (what works in general?)

Architecture + hyperparameter space

Warm starting (what works on *similar* tasks?)



Architecture + hyperparameter space

Model transfer (reuse on very similar tasks)

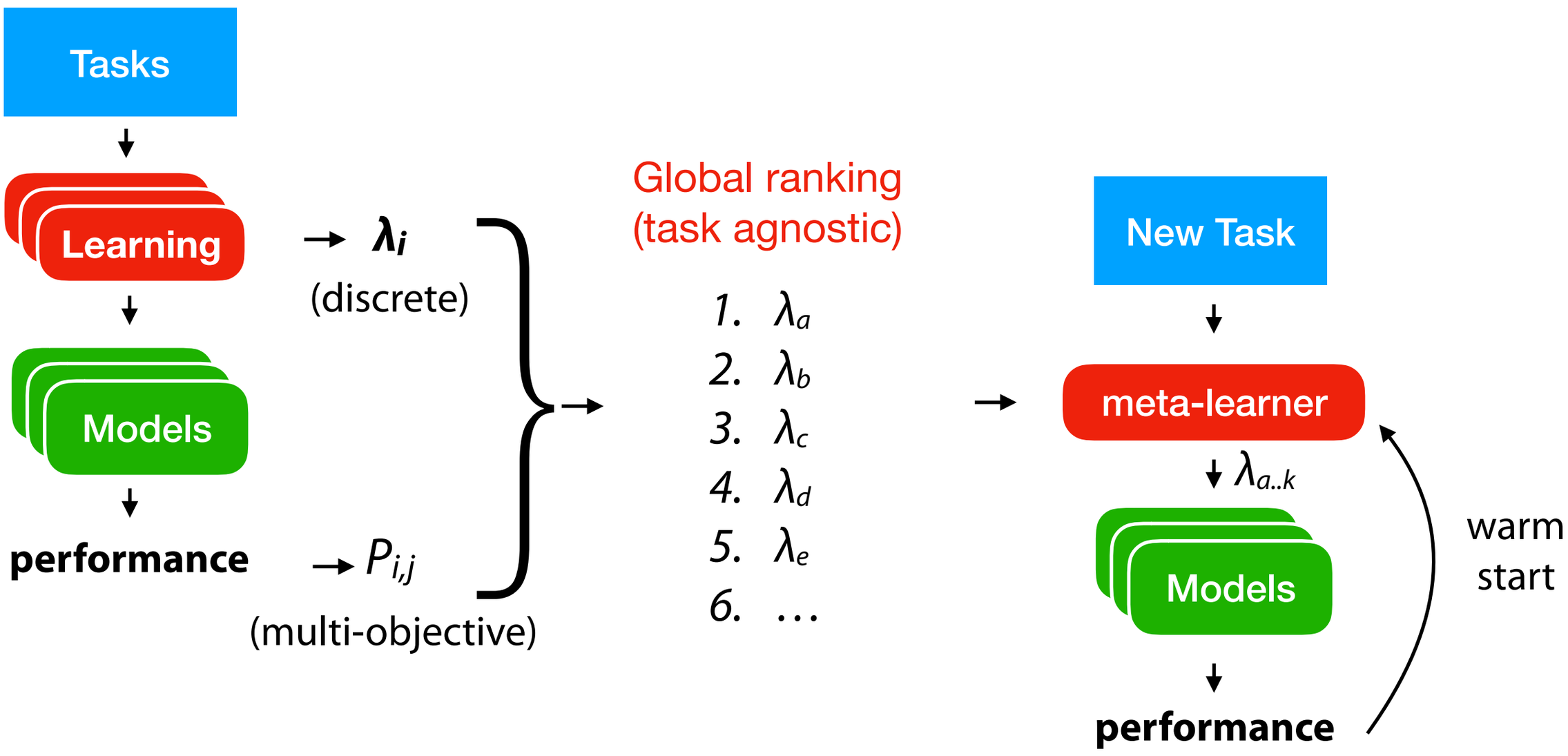
Model parameter space

Leite et al. 2012

Abdulrahman et al. 2018

Model rankings / portfolios

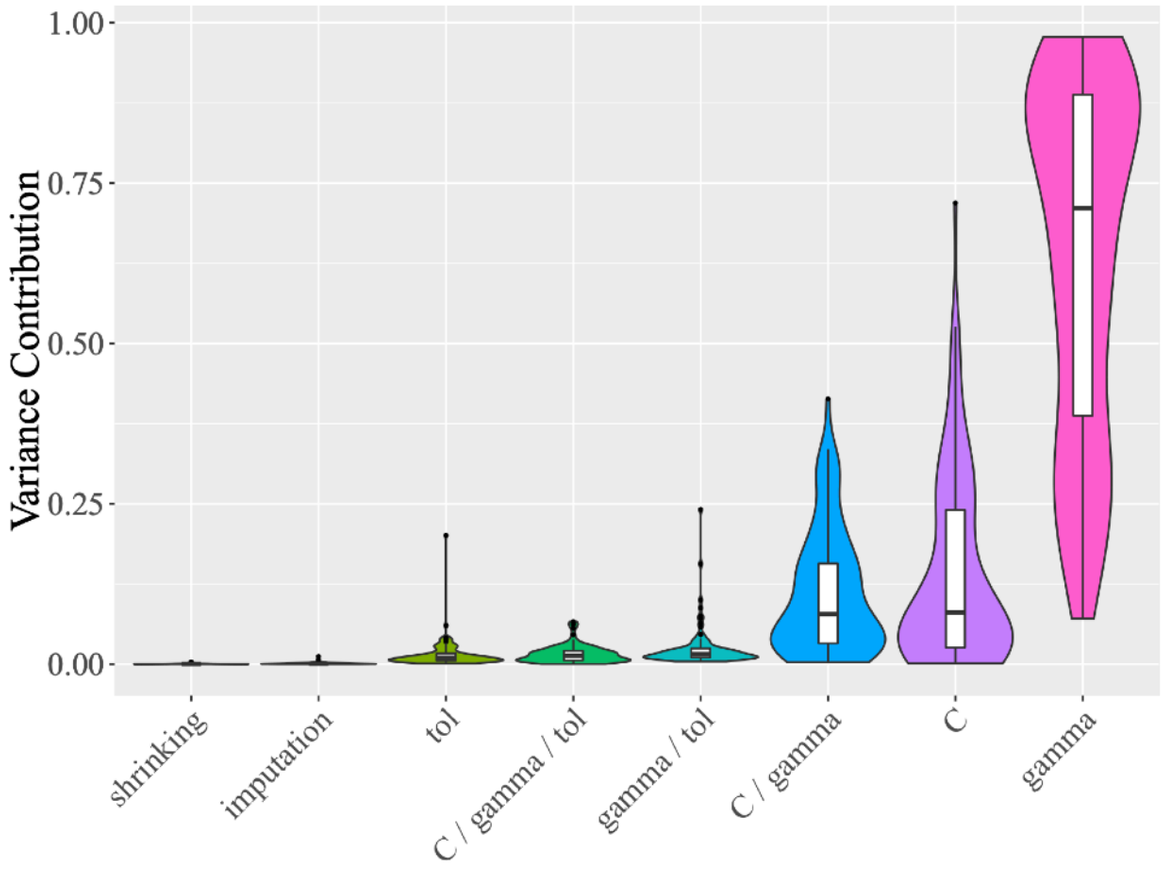
- Discretize the search space, build a *global ranking*, recommend the top-K
- Can be used as a *warm start* for optimization techniques
  - E.g. Bayesian optimization, evolutionary techniques,…



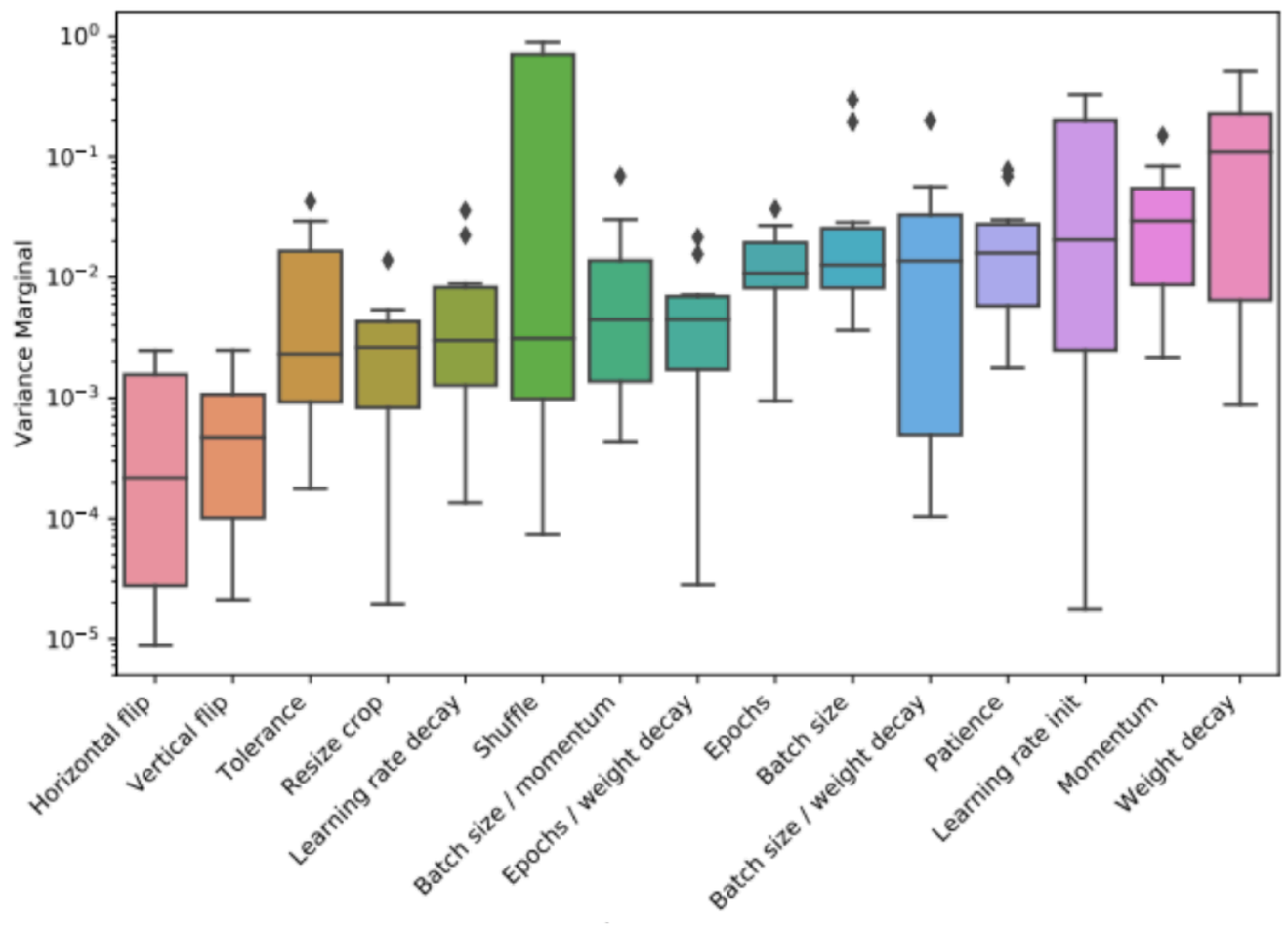
[1] van Rijn & Hutter 2018

Hyperparameter importance

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



SVM (RBF)



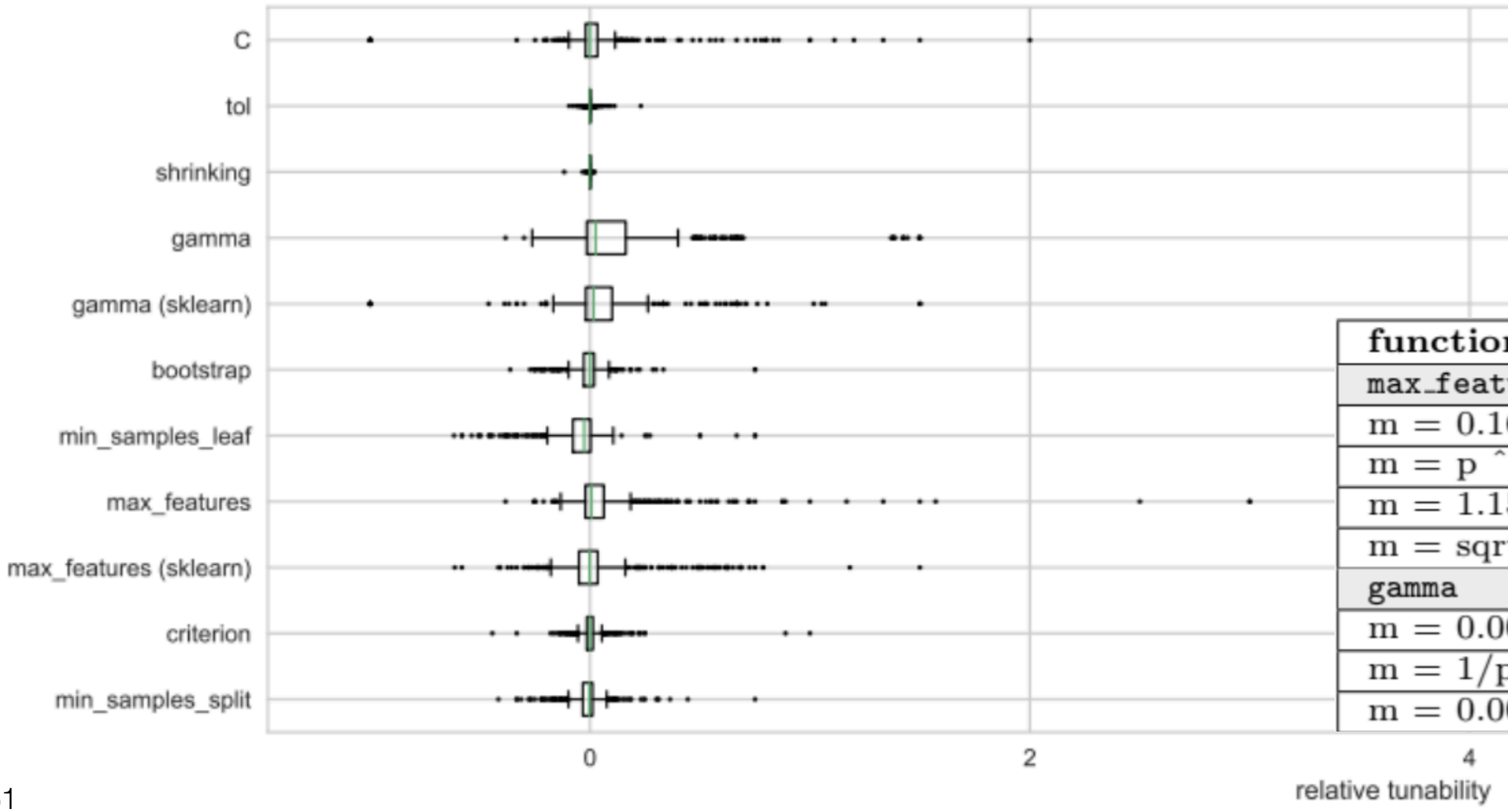
ResNets for image classification

[1] van Rijn & Hutter 2018
[2] Probst et al. 2018
[3] Weerts et al. 2018
[4] van Rijn et al. 2018

Hyperparameter importance

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

- **Tunability** *[2,3,4]*
  Learn good defaults, measure improvement from tuning over defaults



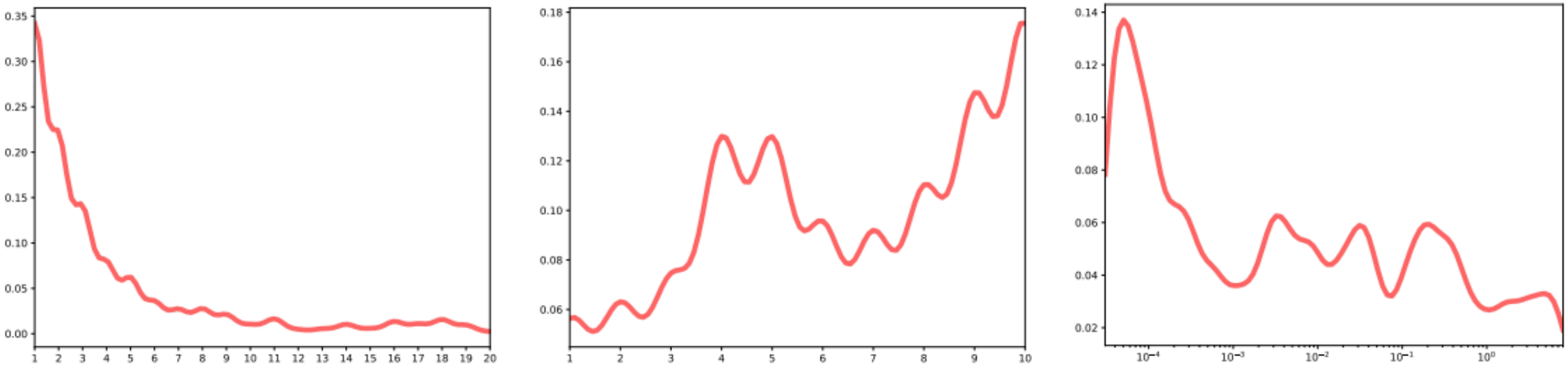
function	RMSE
`max_features`	
m = 0.16*p	21.64
m = p ^0.74	23.13
m = 1.15^sqrt(p)	24.33
m = sqrt(p)	41.38
`gamma`	
m = 0.00574*p	1.25
m = 1/p	1.24
m = 0.006	1.27

van Rijn & Hutter 2018

Wistuba et al. 2015

Hyperparameter priors

- Select hyperparameters that cause variance in the evaluations.
  Learn priors for hyperparameter tuning (e.g. Bayesian optimization)
- Use them to focus on interesting regions (or exclude bad regions)



(a) RF: min. samples per leaf

(b) Adaboost: max. depth of tree

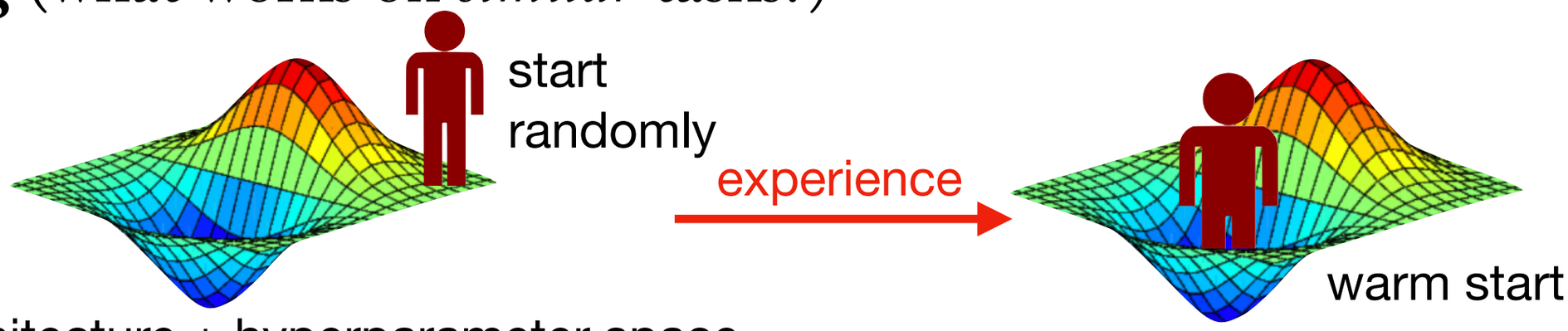
(c) SVM (RBF kernel): gamma

Priors (KDE) for the most important hyperparameters

How to learn how to learn?

Search space design (what works in general?)

Warm starting (what works on *similar* tasks?)



Model transfer (reuse on very similar tasks)

Meta-features

[1] Vanschoren 2018
[2] Rivolli et al 2019
[3] Kim et al. 2017
[4] Achille et al. 2019
[5] Zamir et al. 2018

- Numeric values that describe a certain task
  - Resulting vector allows to compute a distance between task
- **Hand-crafted (interpretable) meta-features** [1,2]
  - **Number of** instances, features, classes, missing values, outliers,…
  - **Statistical:** skewness, kurtosis, correlation, covariance, sparsity, variance,…
  - **Information-theoretic**: class entropy, mutual information, noise-signal ratio,…
  - **Model-based**: properties of simple models trained on the task
  - **Landmarkers**: performance of fast algorithms trained on the task
  - Domain specific task properties
- **Deep metric learning** [3,4,5]
  - Learn a joint representation (embedding) for set of tasks (e.g. image datasets)
    - Ground truth similarity can be based on brute-force evaluation (taskonomy)

Meta-models

[1] Brazdil et al. 2009, Lemke et al. 2015

[2] Sun and Pfahringer 2013, Pinto et al. 2017

[3] Sanders and C. Giraud-Carrier 2017

[4] Yang et al. 2018

- *Learn* direct mapping between meta-features and $P_{i,j}$
  - Zero-shot meta-models: predict best λ_i given meta-features [1]

  - Ranking models: return ranking $\lambda_{1..k}$ [2]

  - Predict portfolio of algorithms / configurations [3]

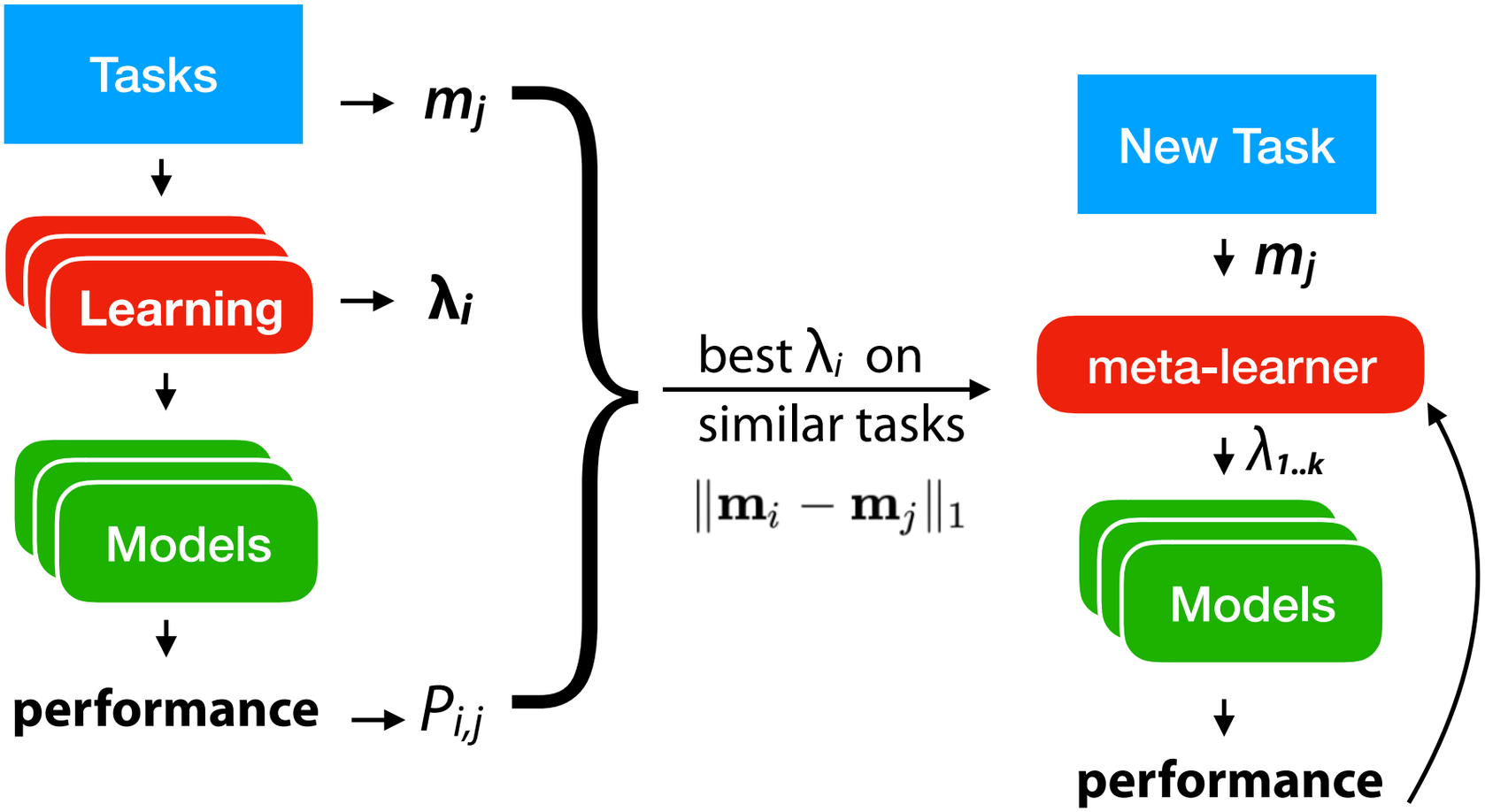
  - Predict performance / runtime for given Θ_i and task [4]

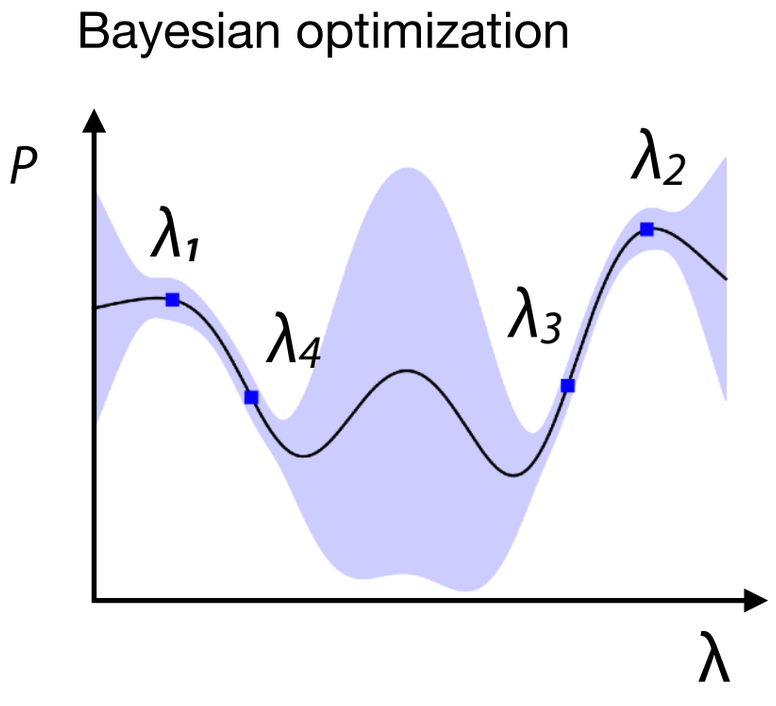
- Can be integrated in larger AutoML systems: warm start, guide search,…

Feurer et al. 2015

Warm-started Bayesian optimization

- Find k most similar tasks based on meta-features, warm-start search with best λ_i
  - Auto-sklearn: Warm-started Bayesian optimization
    - Meta-learning yields better models, faster
    - Winner of AutoML Challenges



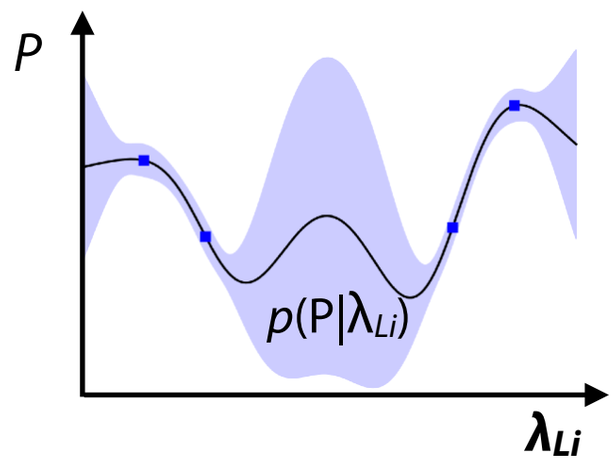


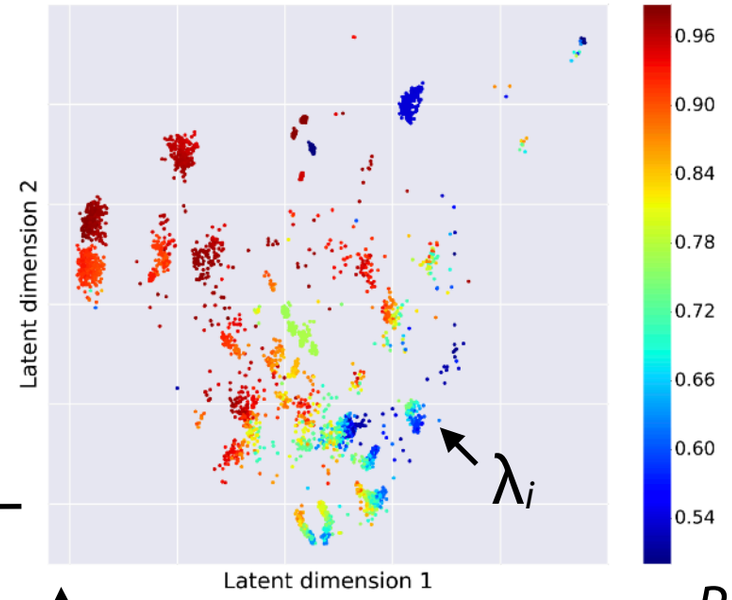
Fusi et al. 2017

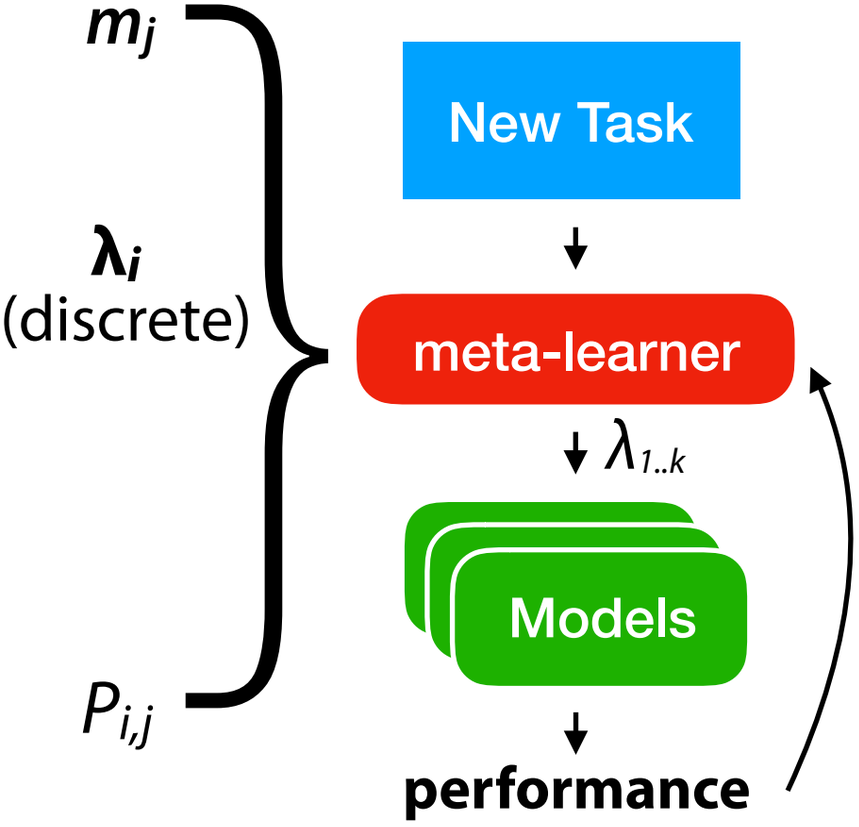
Recommender systems

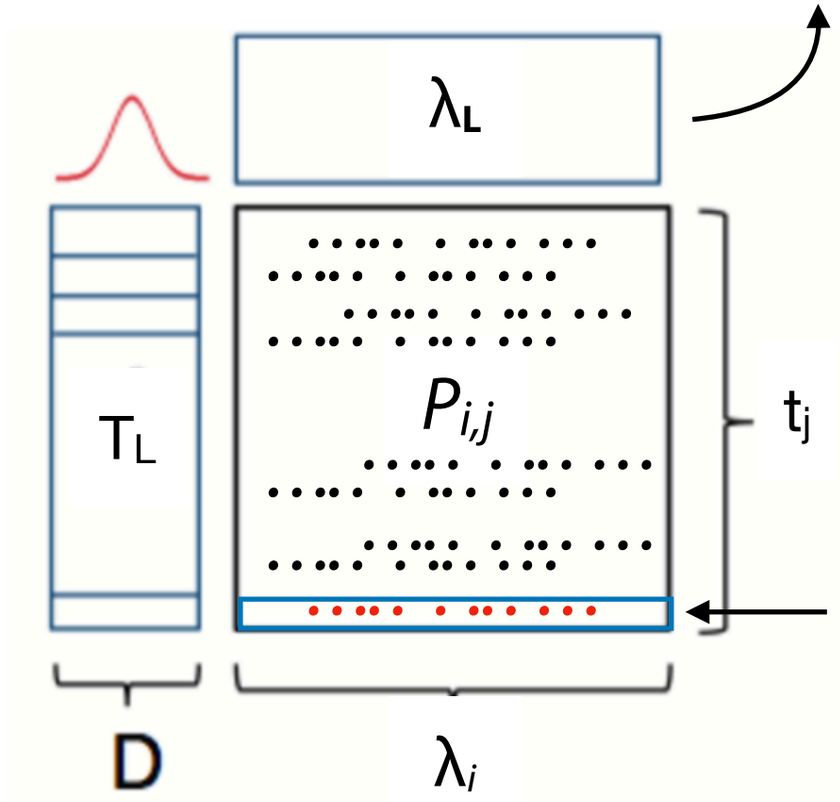
- Collaborative filtering: configurations λ_i are `rated' by tasks t_j

- Use matrix factorization to learn a low-dim. latent representation for tasks and configurations
- Do BayesOpt in the latent configuration space
- Solve cold-start problem by warm-starting with best $\lambda_{1..k}$









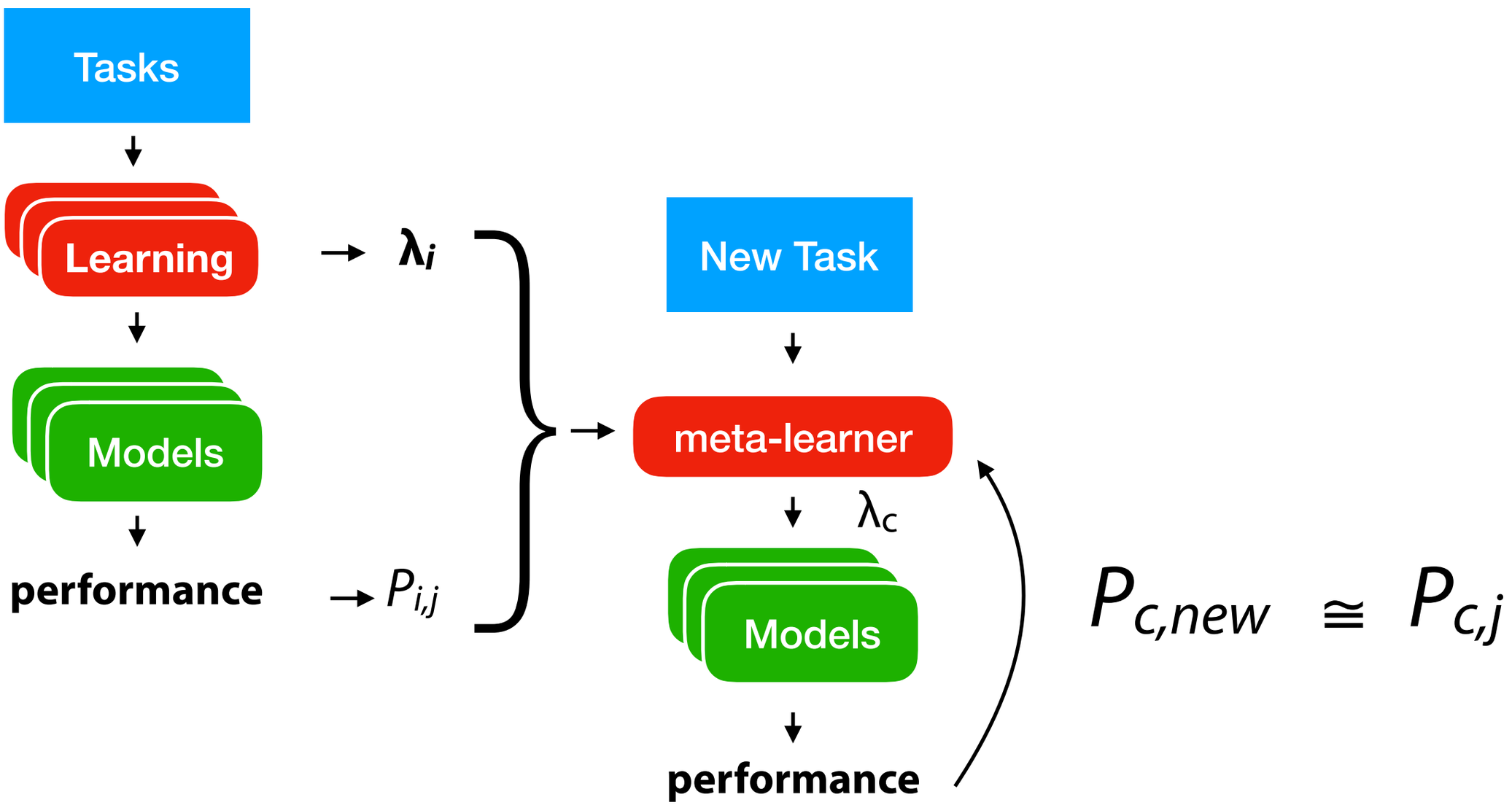
latent representation

t_{new} warm-started with $\lambda_{1..k}$

Leite et al. 2012

Learning task similarity

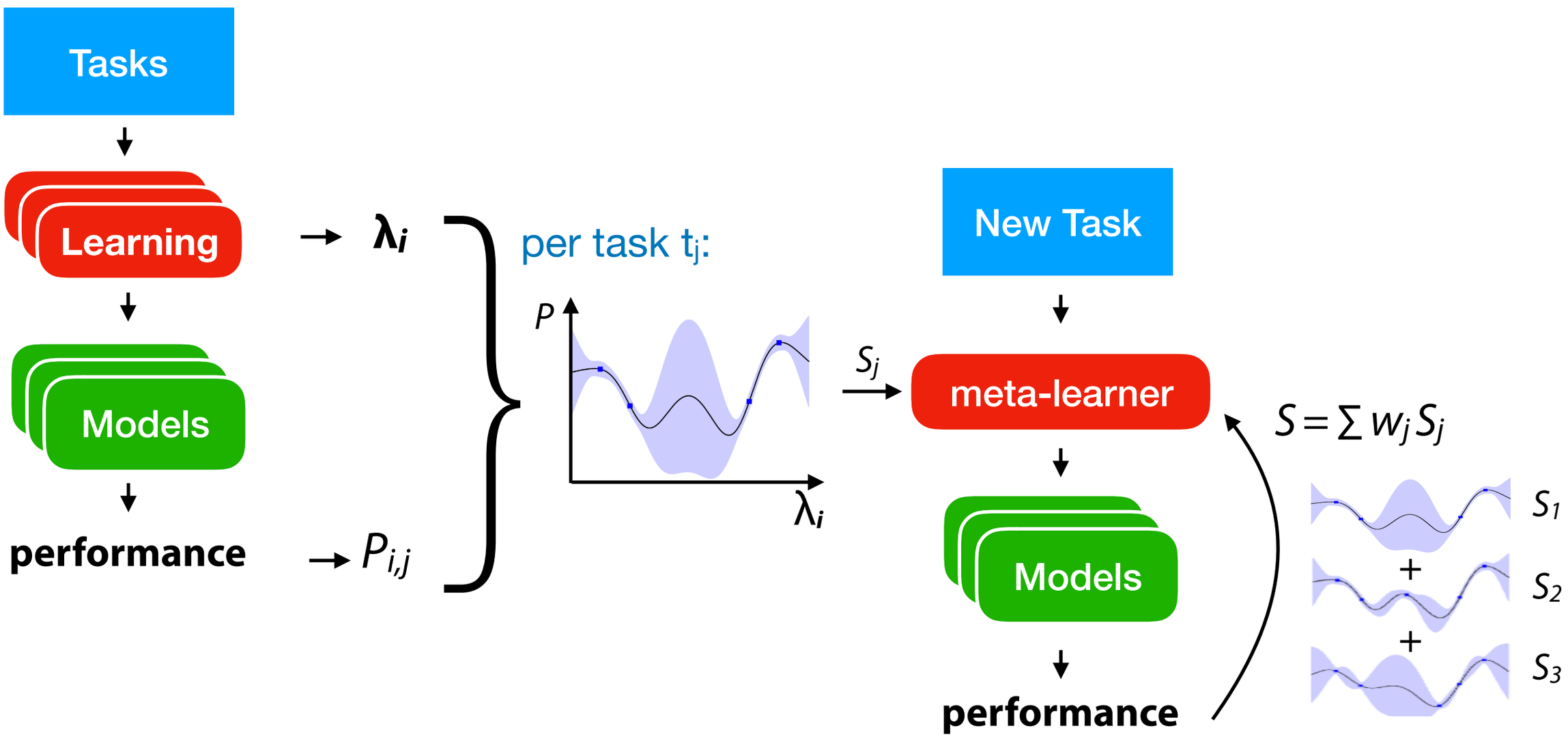
- Experiments on the *new* task can tell us how it is similar to *previous* tasks
- **Task *j* is *similar*** to new task if observed *performance* of configurations is similar
- Use this to recommend configurations that worked well on task j *(active testing)*



Surrogate model transfer

[1] Wistuba et al. 2018
[2] Feurer et al. 2018
[3] Manolache & Vanschoren, 2019

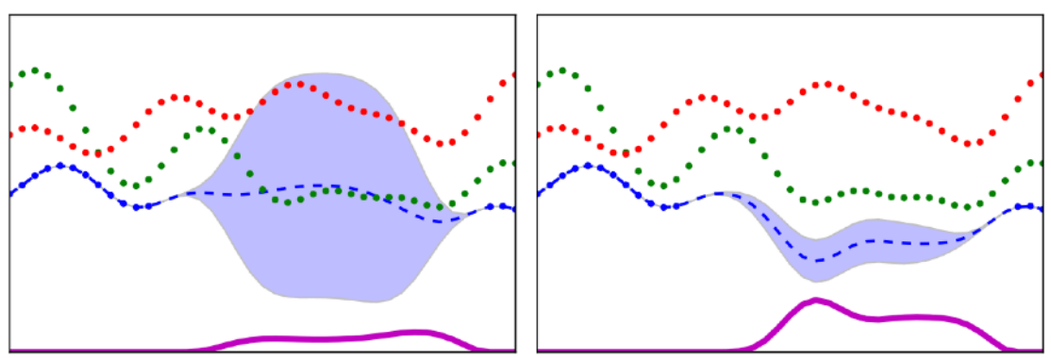
- If task j is *similar* to the new task, its surrogate model S_j will likely transfer well
- Sum up all S_j predictions, weighted by task similarity (as in active testing)[1]
- Surrogate model for new task is weighted sum of surrogates of previous tasks, *weighted by how well they recommend configurations for the new task*[2,3]



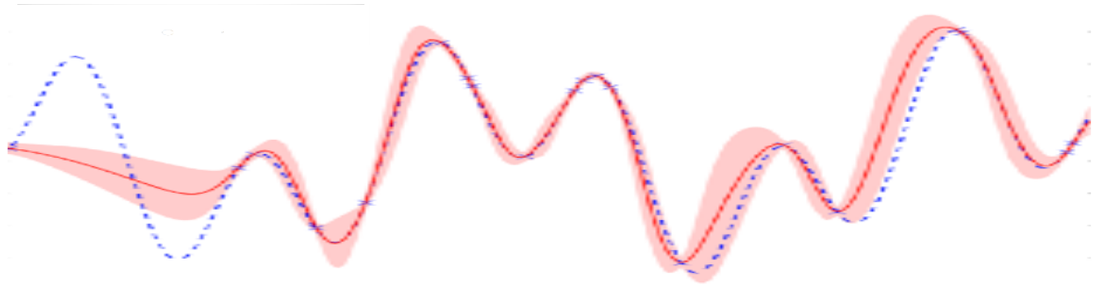
Multi-task Bayesian optimization

[1] Swersky et al. 2013
[2] Springenberg et al. 2016
[3] Golovin et al. 2017

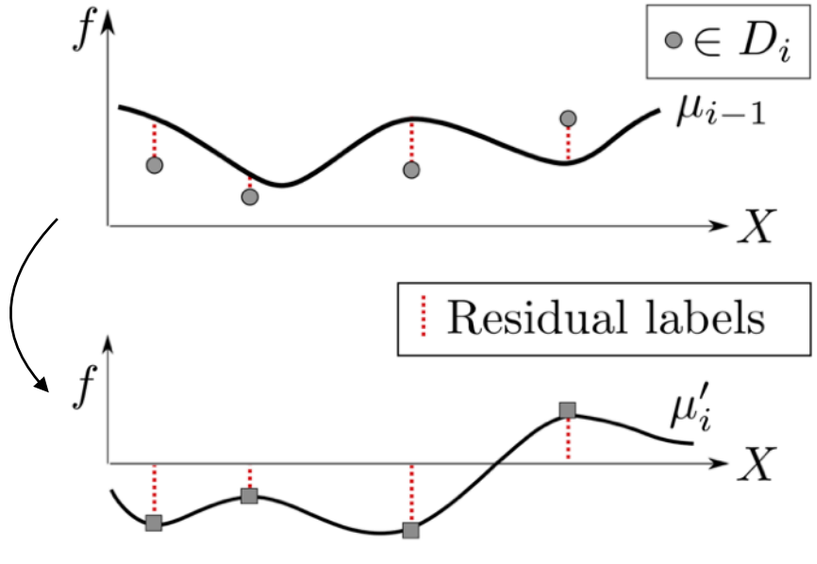
- Consider multiple similar tasks at once (e.g. datasets from different days)
- **Multi-task Gaussian processes:** train surrogate model on t tasks simultaneously[1]
  - If tasks are similar: transfers useful info
  - Not very scalable



- **Bayesian Neural Networks** as surrogate model[2]
  - Multi-task, more scalable



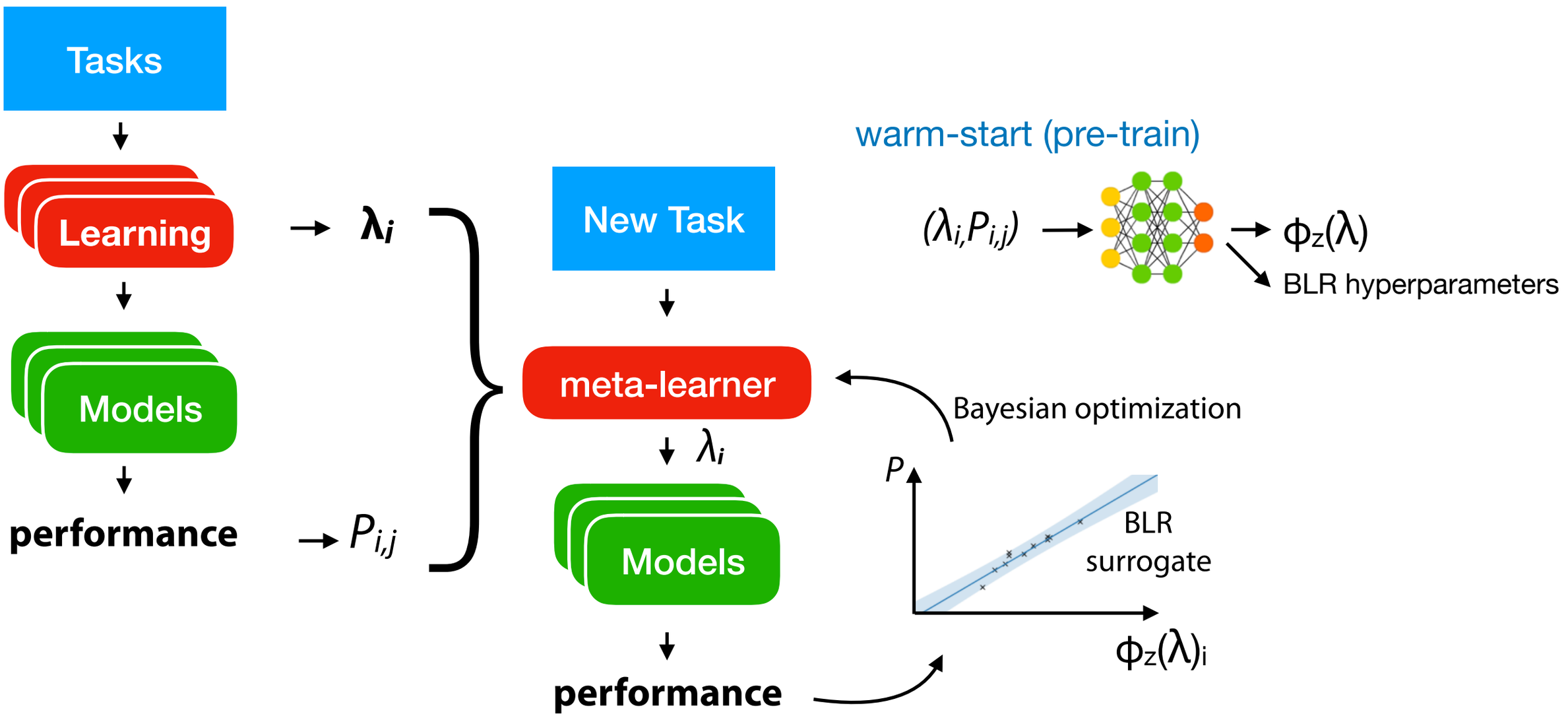
- **Stacking** Gaussian Process regressors (Google Vizier)[3]
  - Continual learning (sequential similar tasks)
  - Transfers a prior based on residuals of previous GP



Perrone et al. 2018

Learn basis expansions for hyperparameters

- Bayesian linear regression (BLR) surrogate model on every task
- Use neural net to learn a suitable basis expansion $\phi_z(\lambda)$ for all tasks
- Scales linearly in # observations, transfers info on configuration space

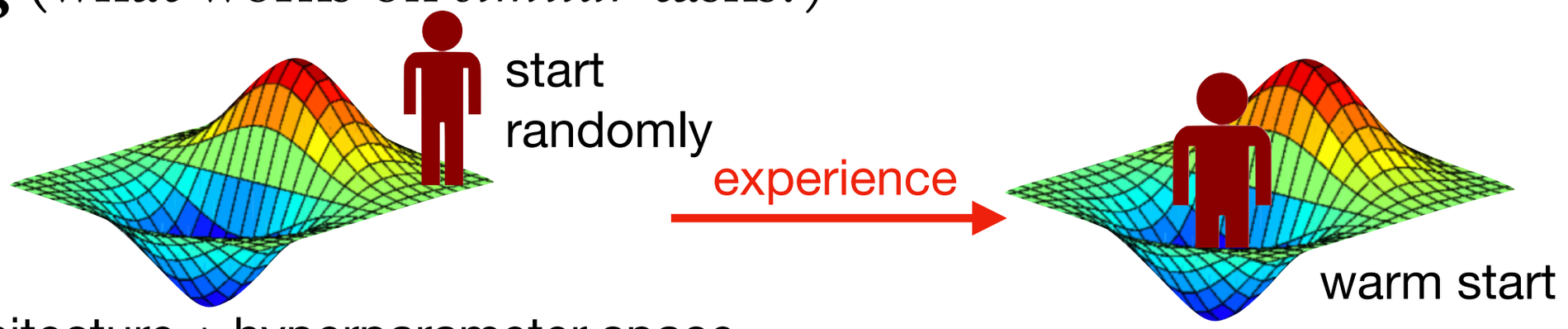


How to learn how to learn?

Search space design (what works in general?)

Architecture + hyperparameter space

Warm starting (what works on *similar* tasks?)



Architecture + hyperparameter space

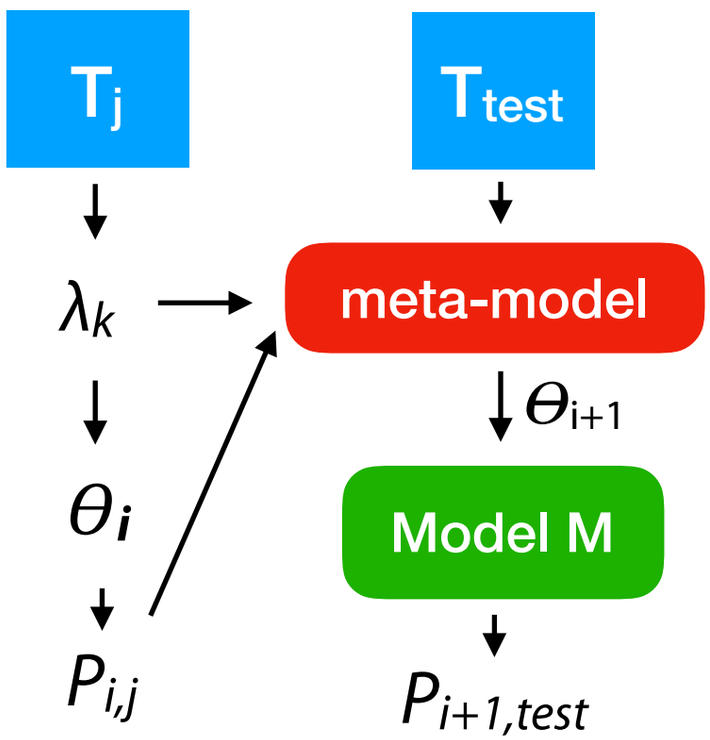
Model transfer (reuse on very similar tasks)

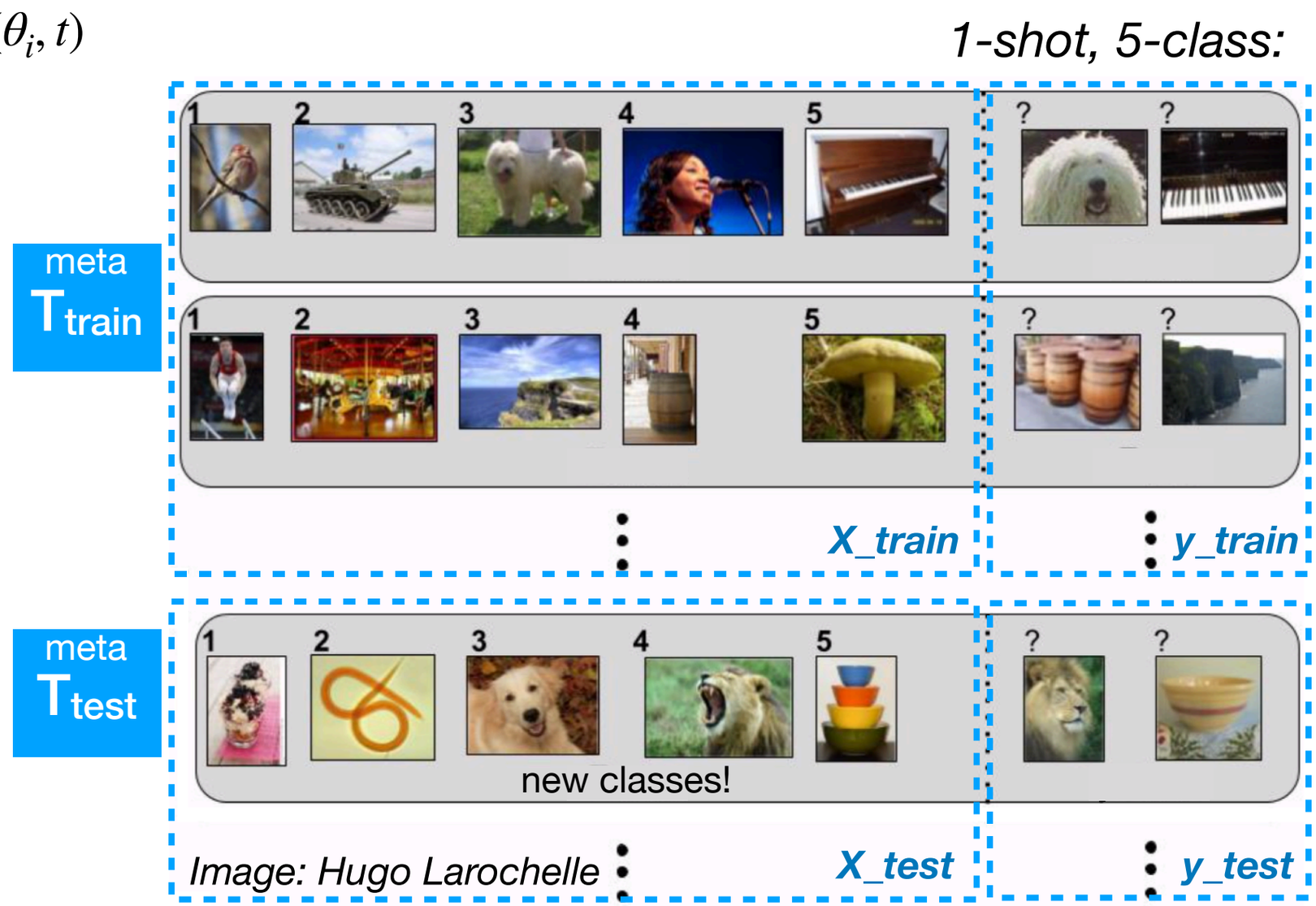
Model parameter space

Example application: Few-shot learning

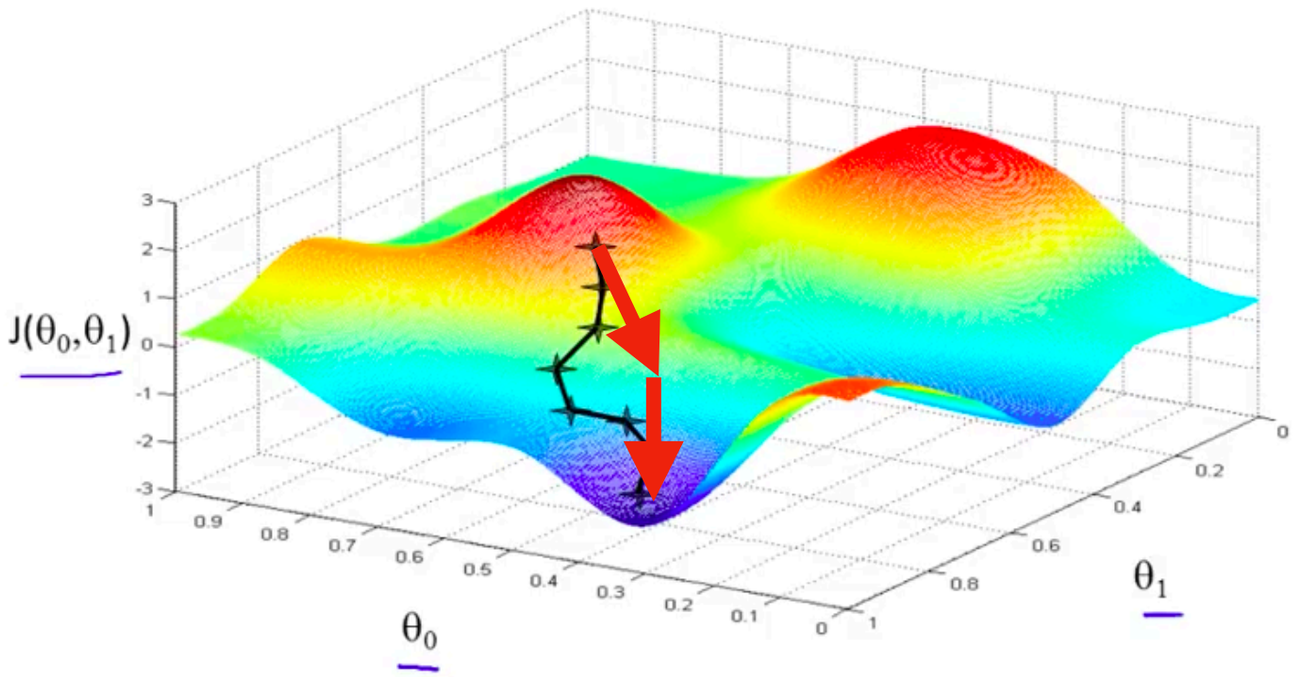
- Learn how to learn from few examples (given similar tasks)
  - Meta-learner must learn how to train a base-learner based on prior experience
    - Parameterize base-learner model and learn the parameters Θ_i

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

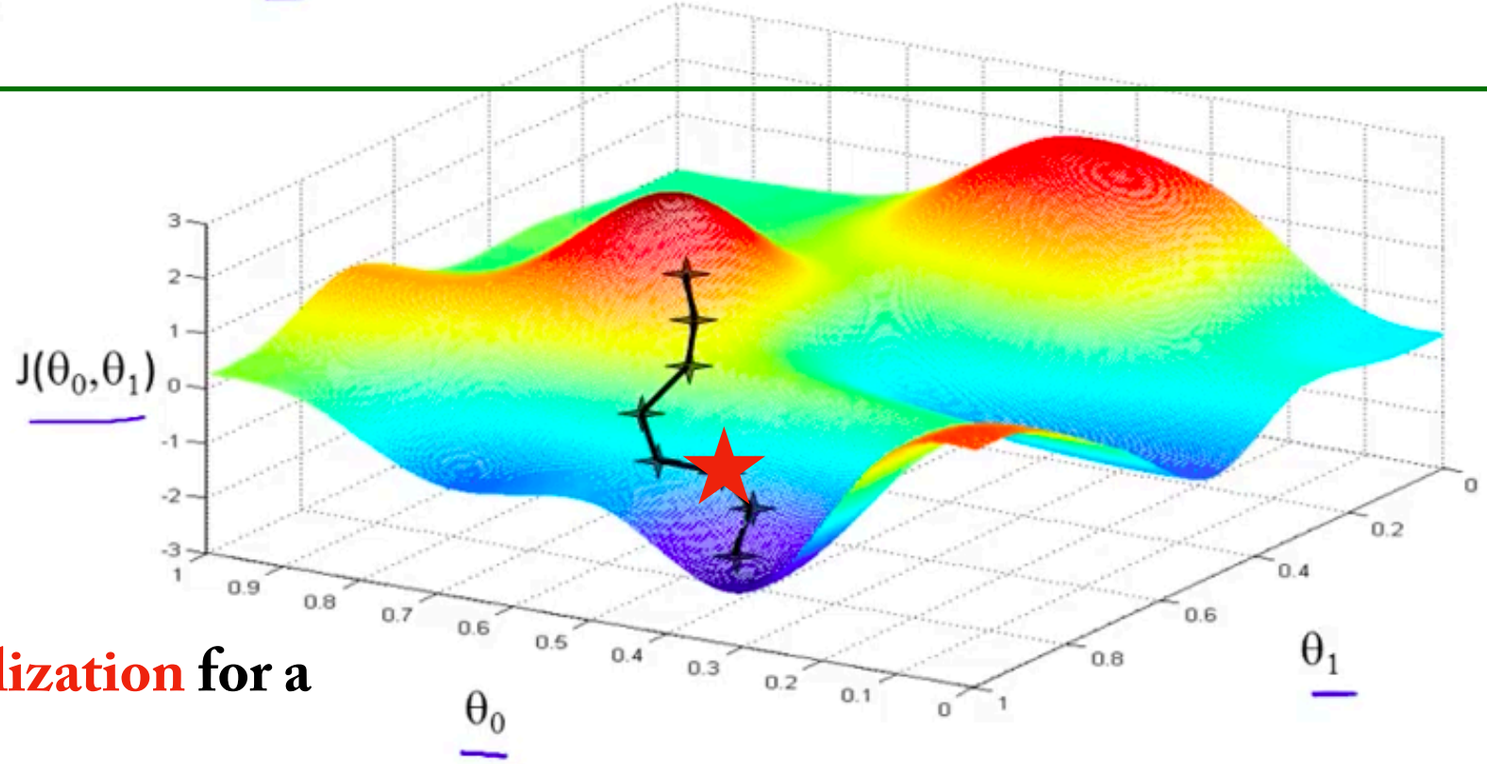




Model transfer (Learning to learn)



Learn and transfer a gradient descent update rule for a group of tasks



Learn and transfer a weight initialization for a group of tasks

[1] Bengio et al. 1995

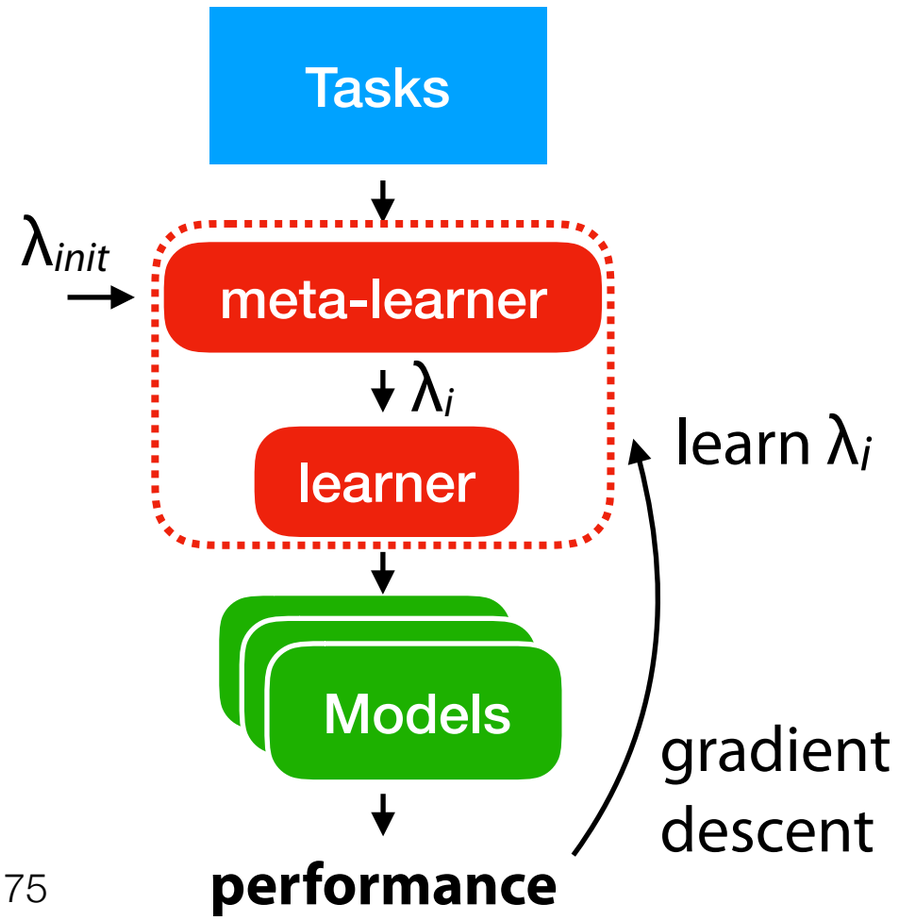
[2] Runarsson and Jonsson 2000

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.

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

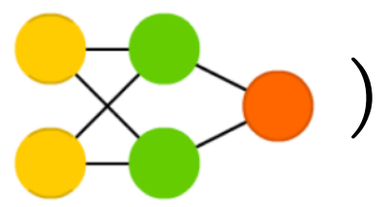
presynaptic activity

learning rate

reinforcing signal

Runarsson and Jonsson

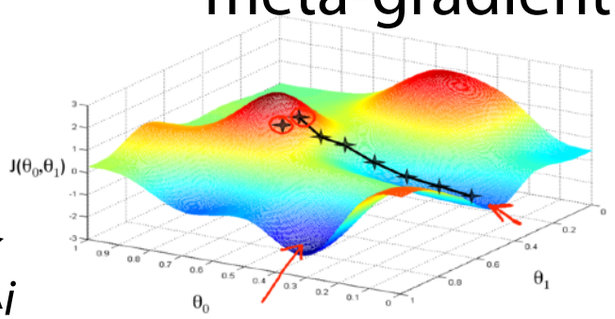
$$\Delta \theta_i = \eta \, (\quad)$$



learning rate

weights λ_i

meta-gradient

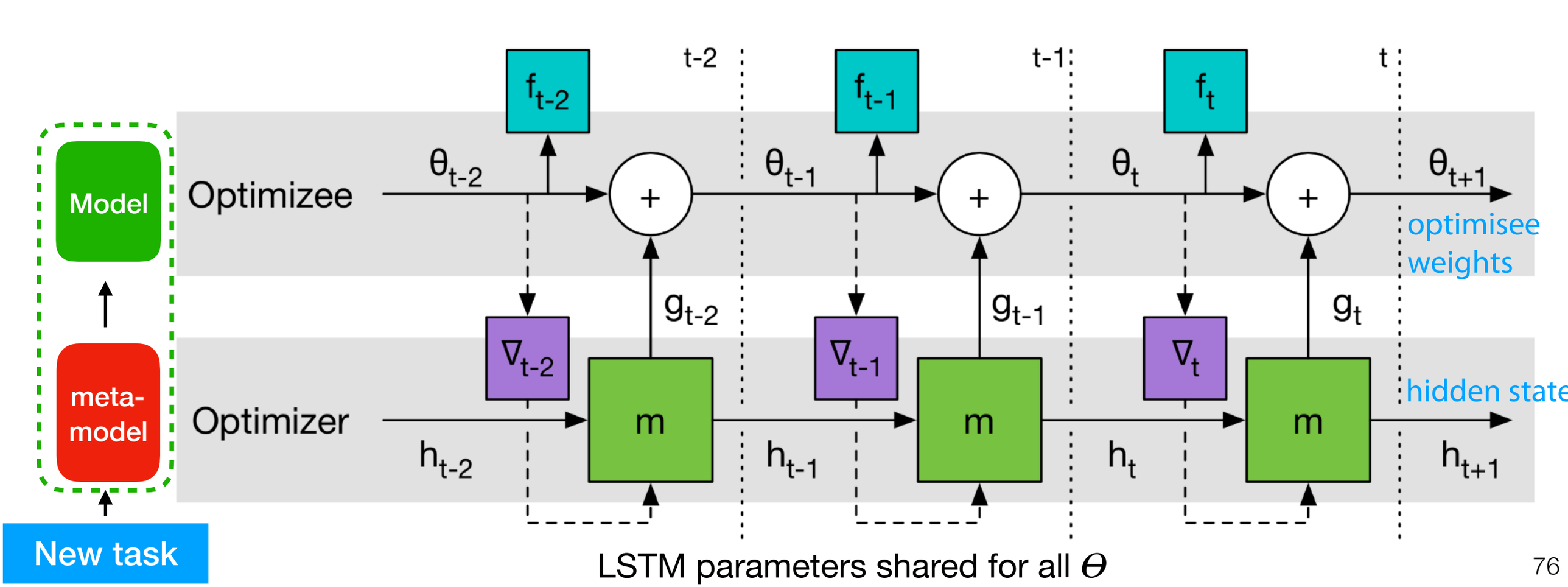


Meta-Learning

[1] Hochreiter 2001
[2] Andrychowicz et al. 2016

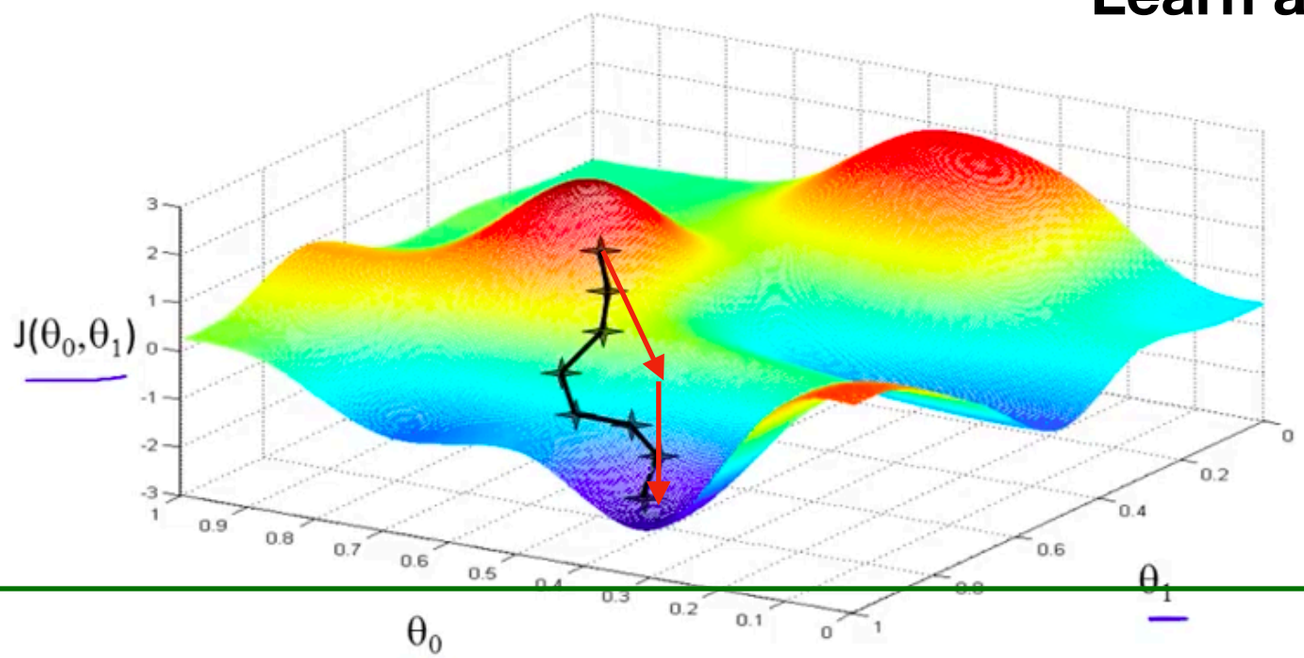
Learning to learn gradient descent by gradient descent

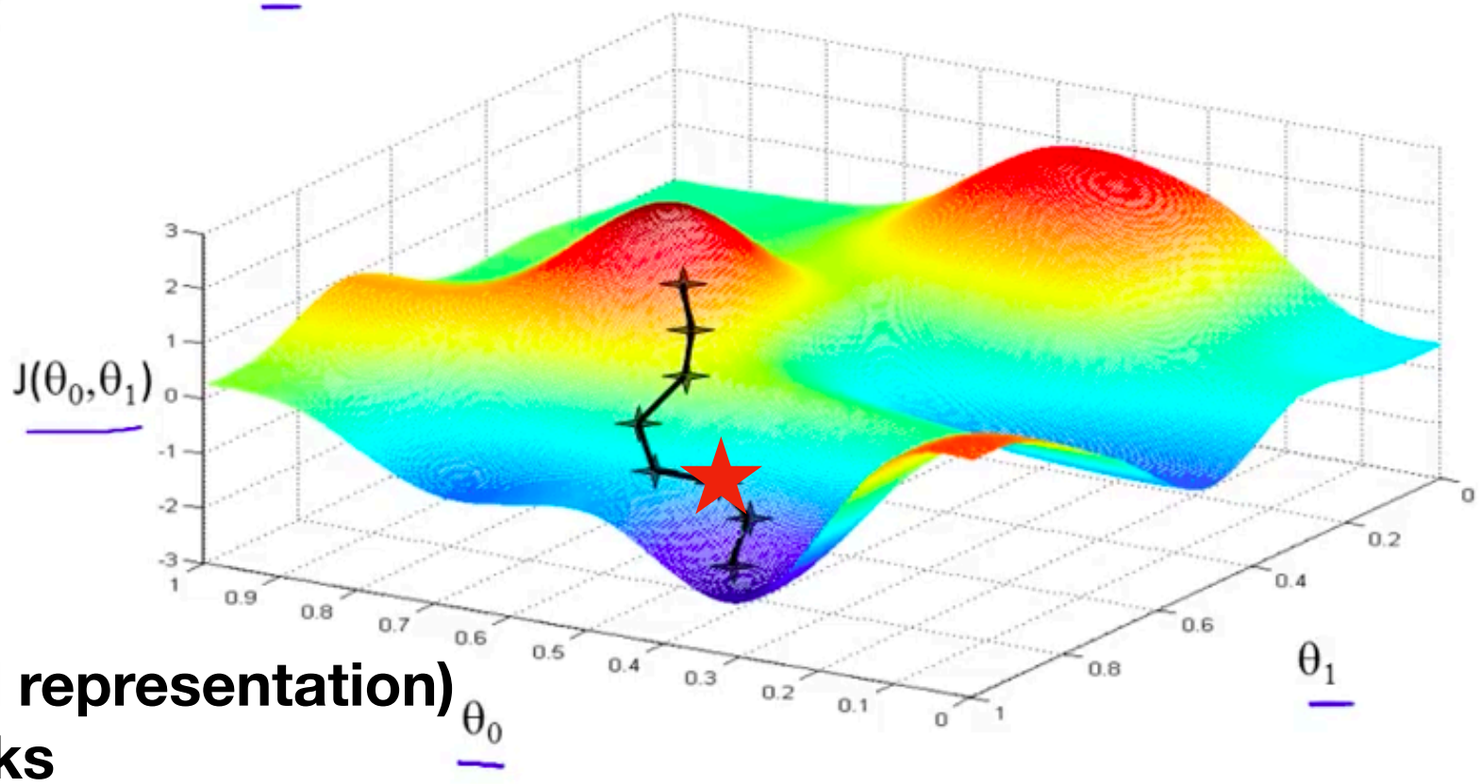
- Replace backprop with a recurrent neural net (LSTM)[1], not so scalable
- Use a coordinatewise LSTM [m] for scalability/flexibility (cfr. ADAM, RMSprop) [2]
  - Optimizee: receives weight update g_t from optimizer
  - Optimizer: receives gradient estimate ∇_t from optimizee
    - Learns how to do gradient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



Model transfer (Learning to learn)

Learn a better gradient update rule for a group of tasks





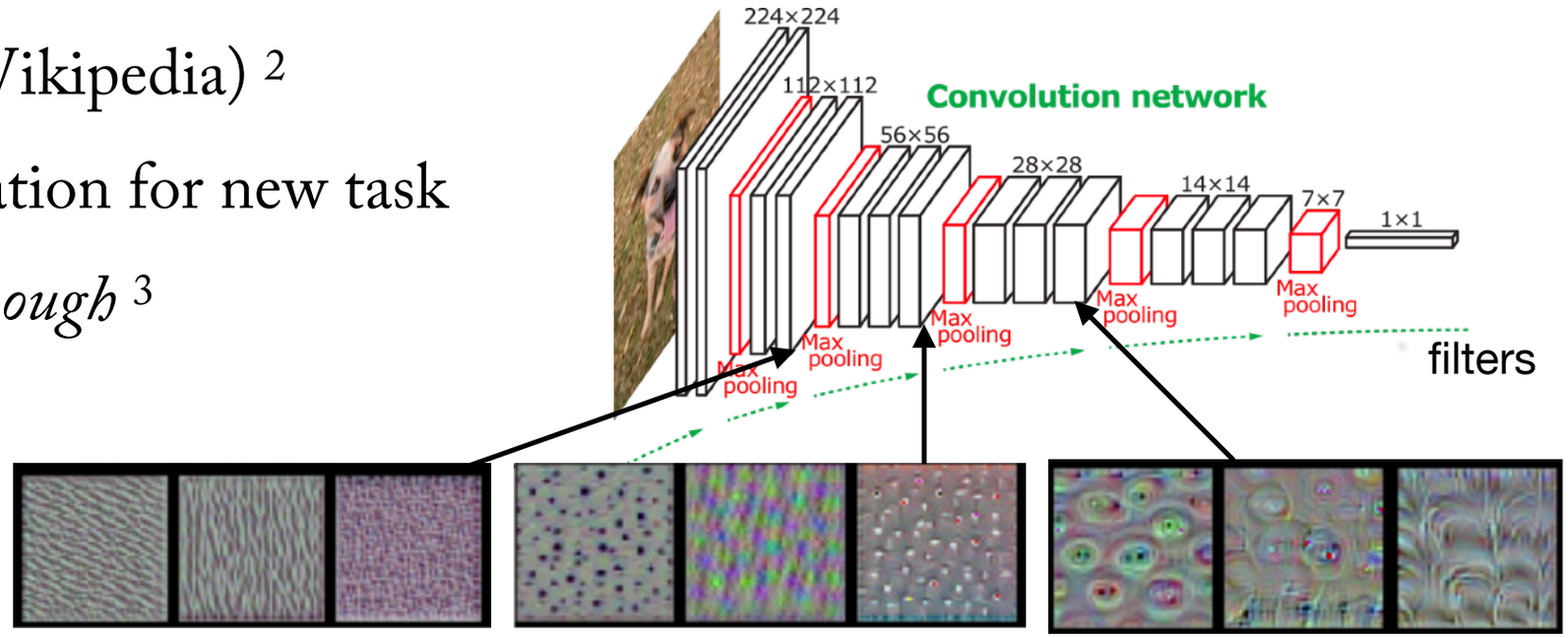
Learn a better initialization (and representation) for a group of tasks

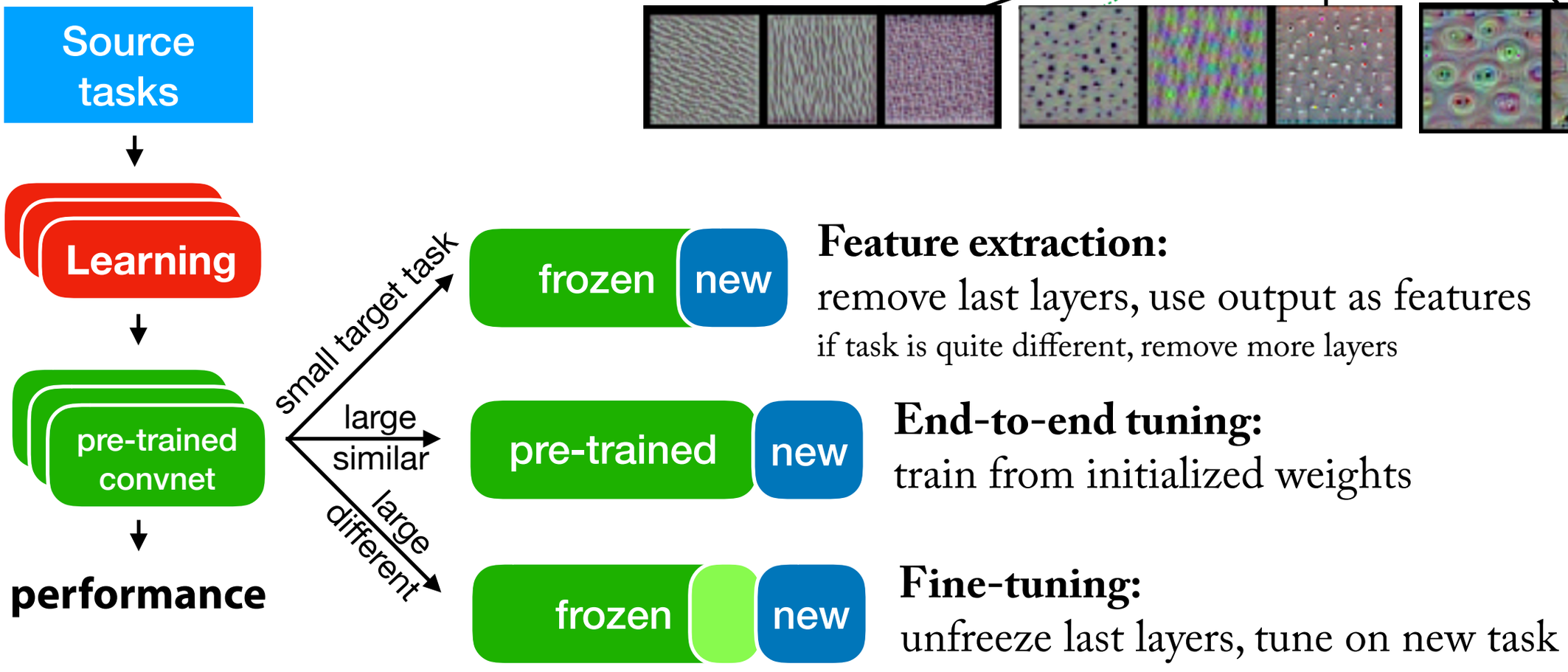
Meta-Learning

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

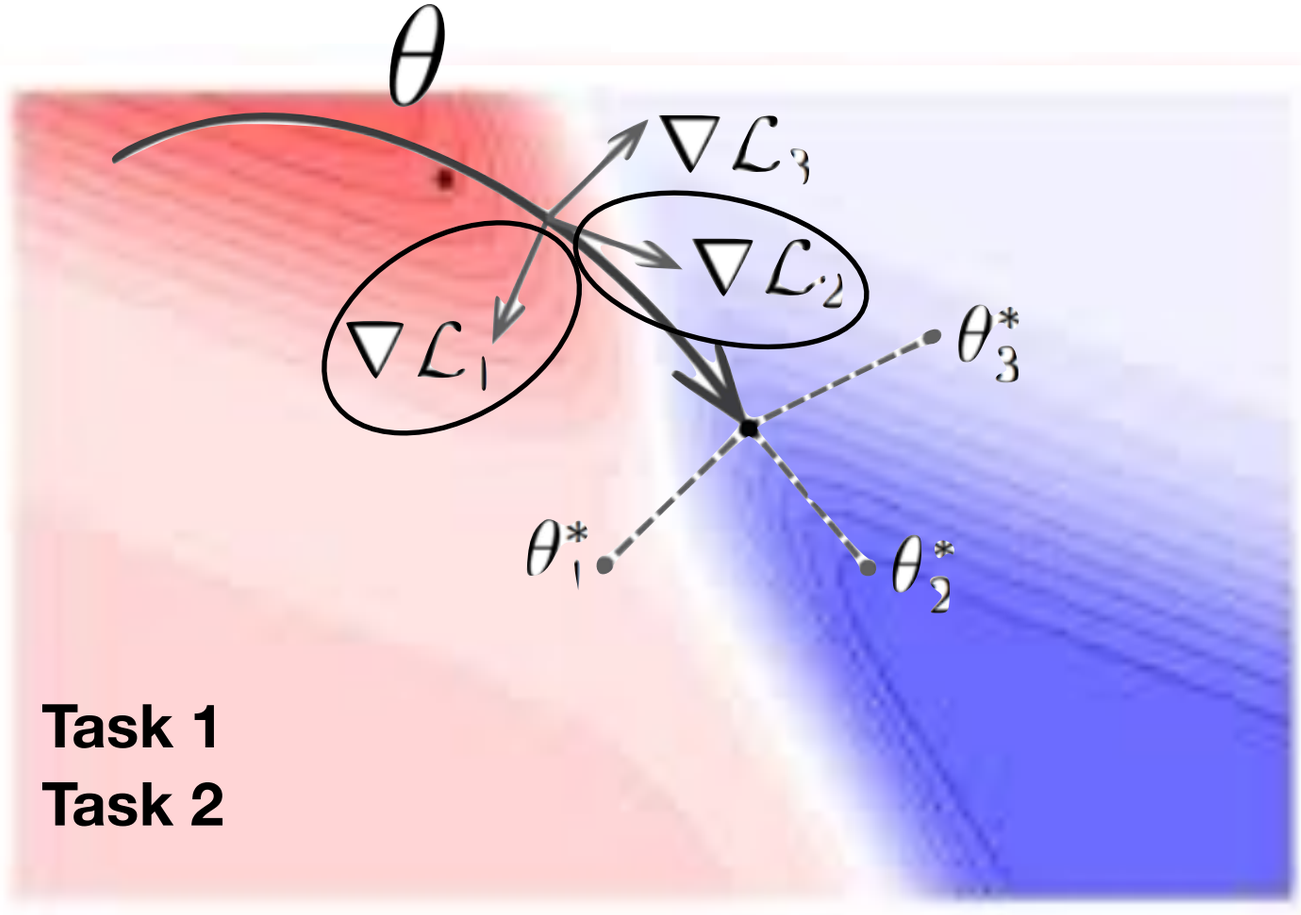
[1] Finn et al. 2017

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



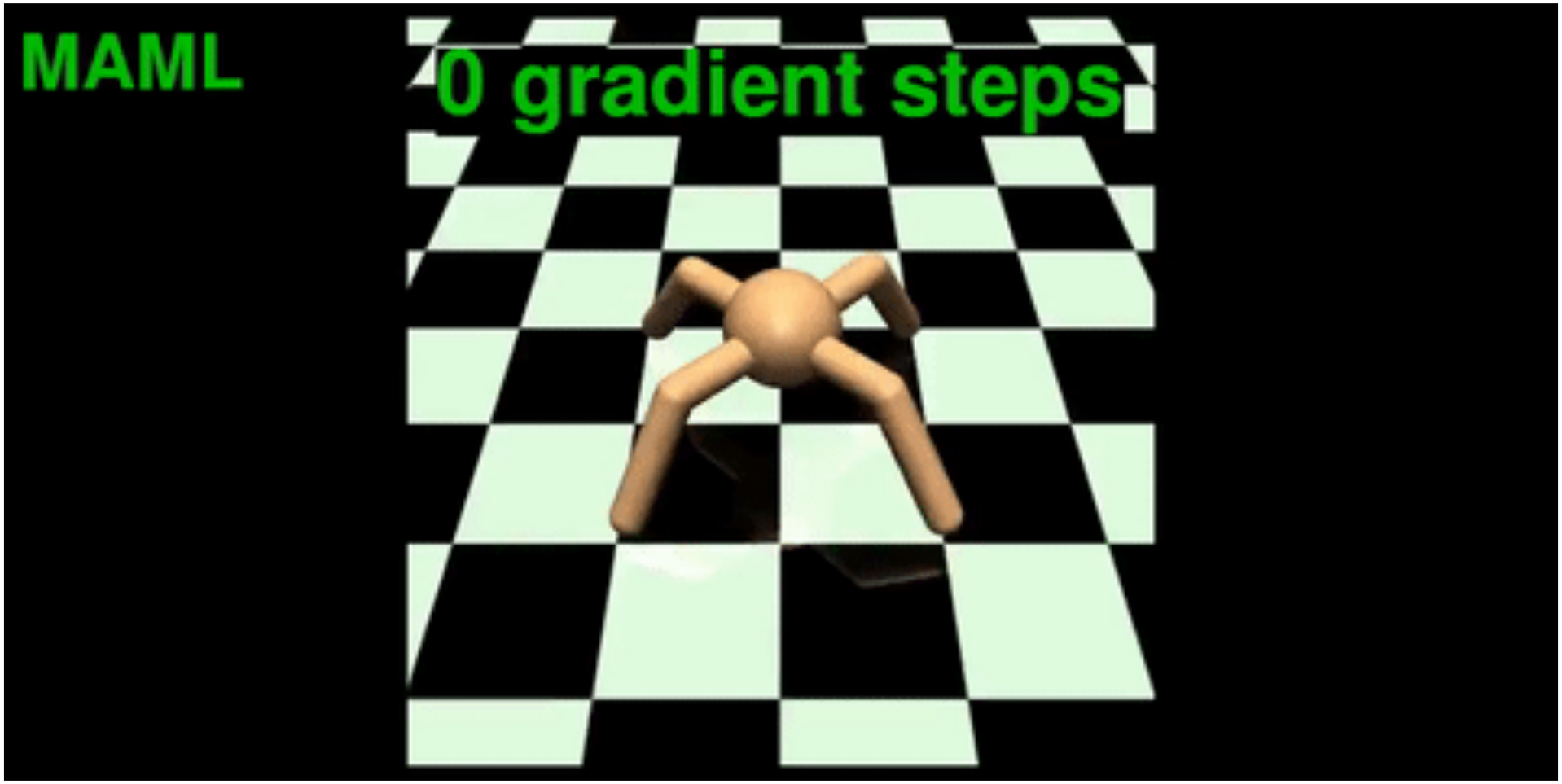
Model-agnostic meta-learning

[1] Finn et al. 2018
[2] Nichol et al. 2018
Finn & Levine 2019

- *Universality* [1]: no theoretical downsides in terms of expressivity when compared to alternative meta-learning models.
- Many variants and applications:
  - 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

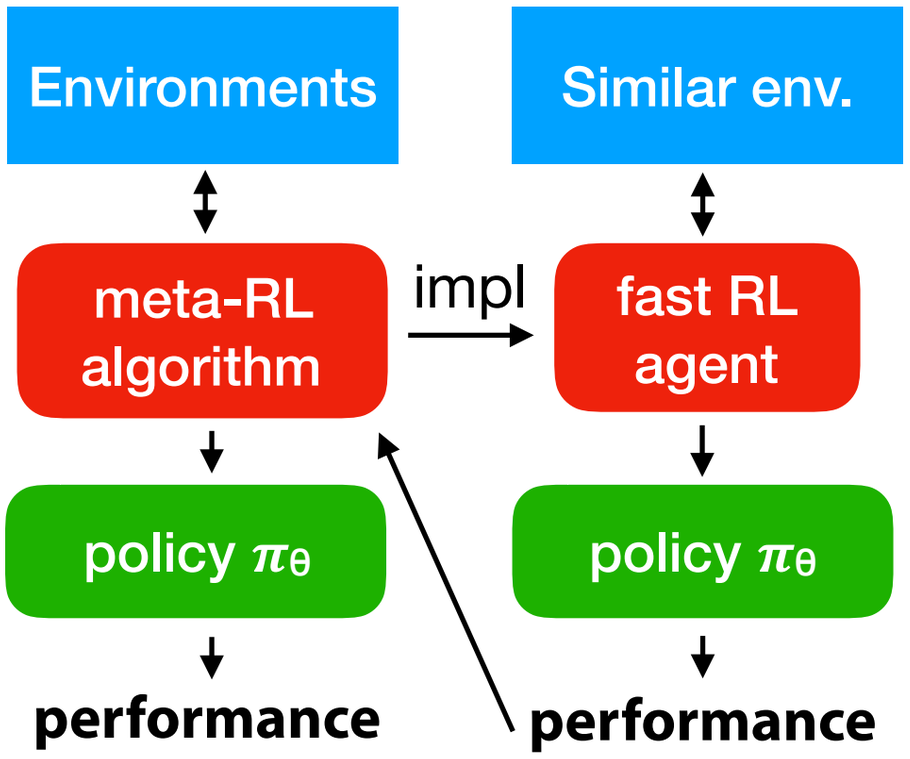
- For reinforcement learning:



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

Meta-reinforcement learning

- 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 of that learner as a reward



- Learning to reinforcement learn [1,2]
  - Use RNN-based deep RL to train a recurrent network on many tasks (slow)
  - Learns to implement a RL agent for a new task that is pre-trained (fast)

Gomez & Vanschoren, NeurIPS 2019

Meta-Reinforcement Learning for NAS

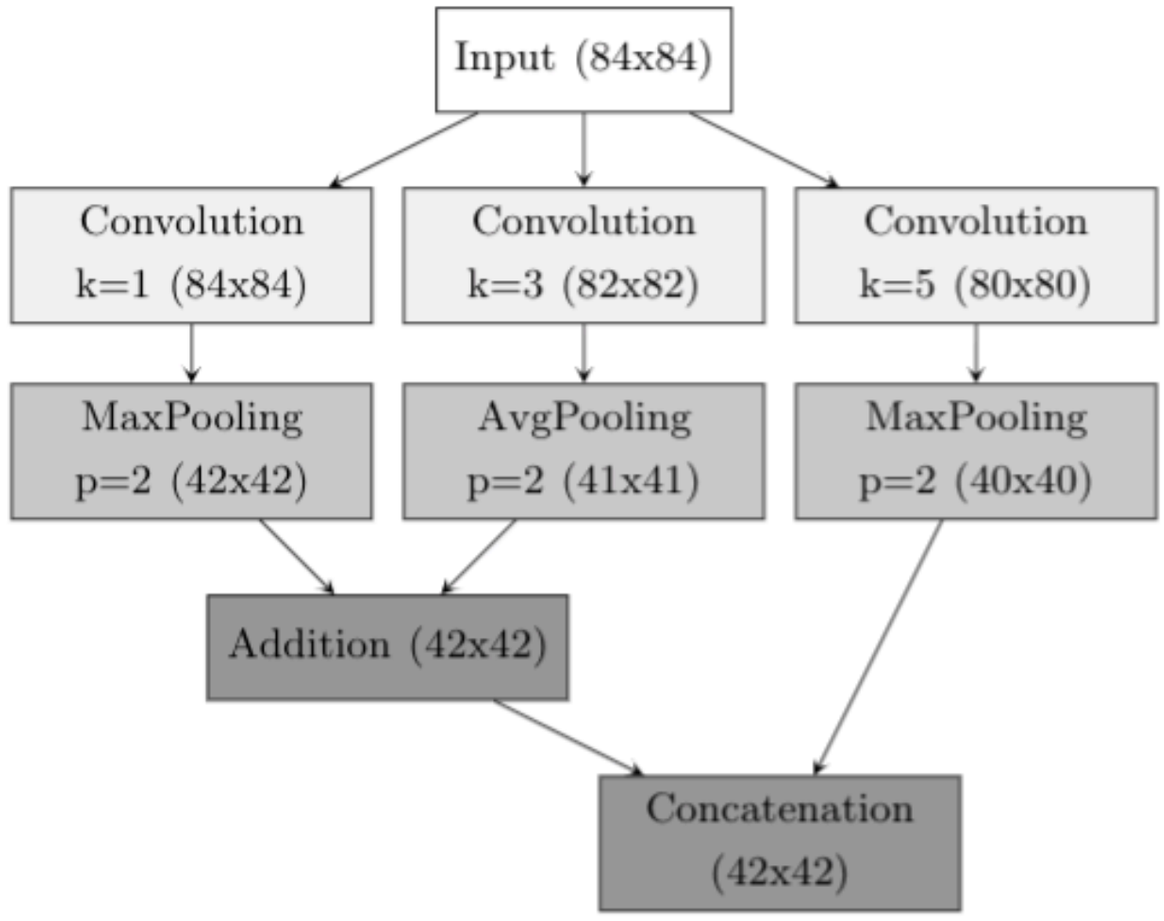
- Train an agent how to build a neural net, across tasks
- Should transfer but also adapt to new tasks

neural 'code'

[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

model created by given 'code'

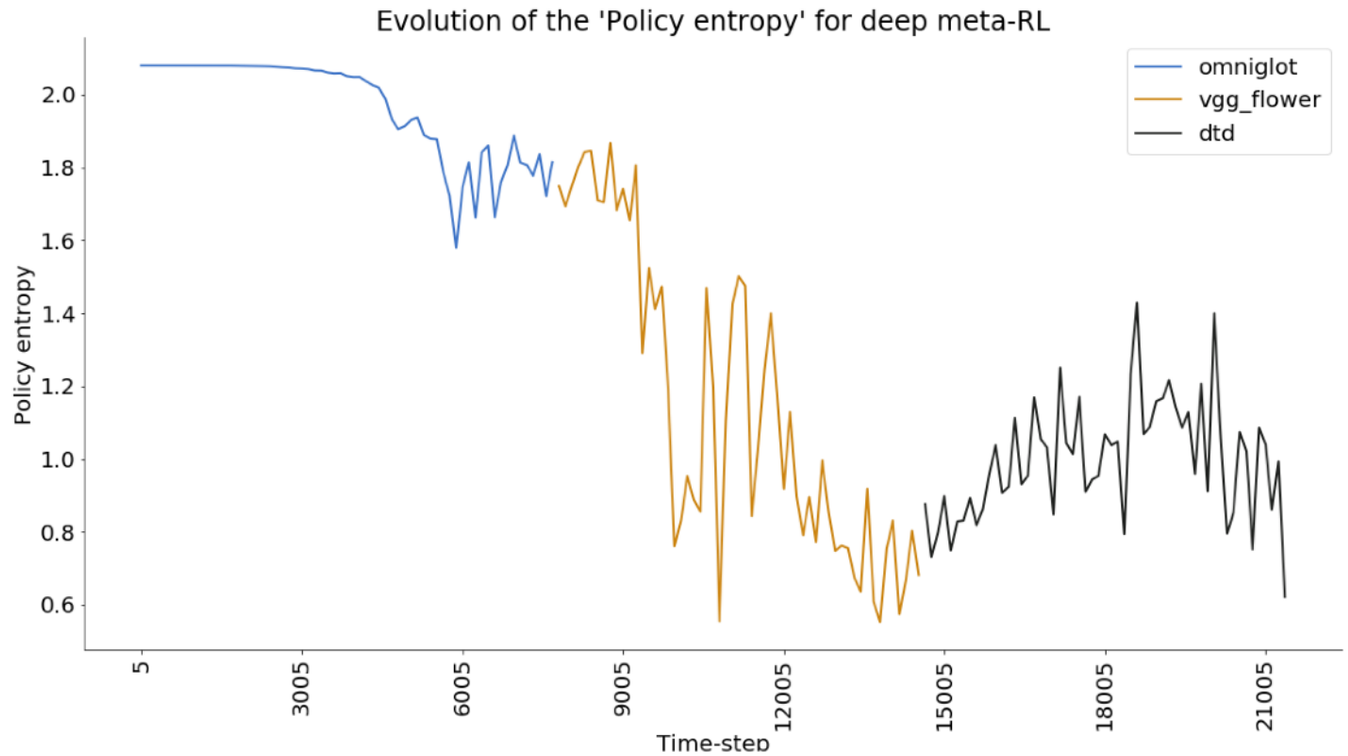


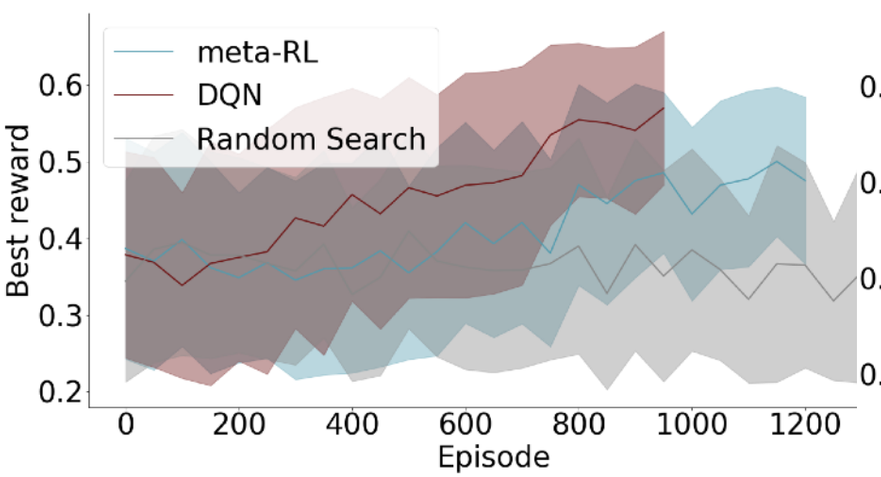
Gomez & Vanschoren, NeurIPS 2019

Meta-Reinforcement Learning for NAS

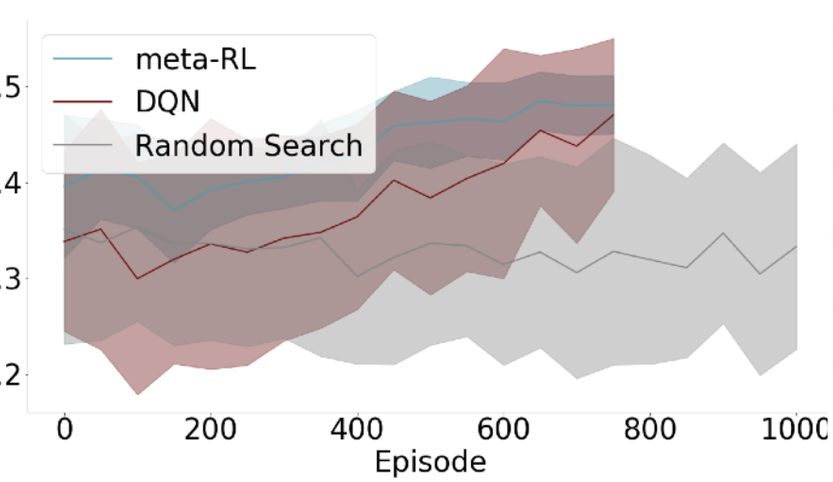
Results on increasingly difficult tasks:

- omniglot
- vgg_flower
- dtd

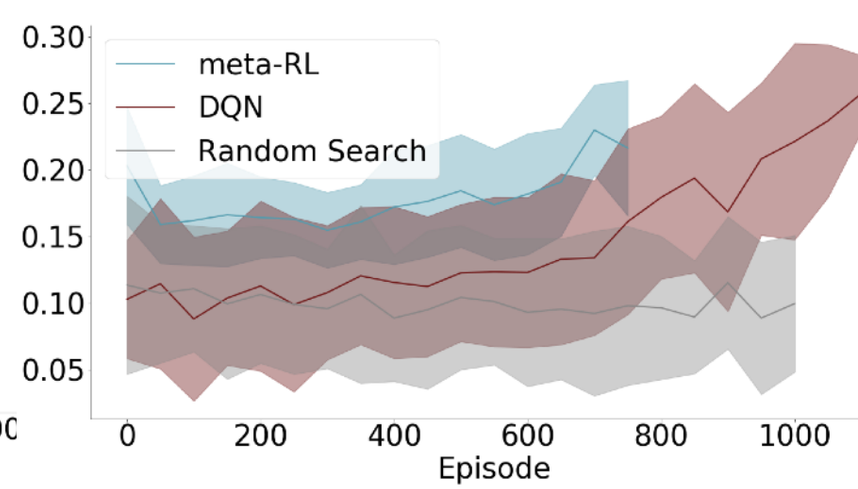




omniglot



vgg_flower



dtd

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