Automated Machine Learning (AutoML)

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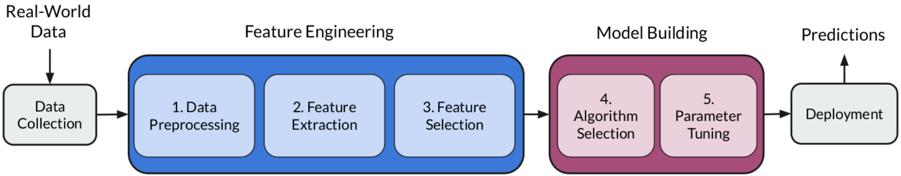
The Course Web Page

https://fid3024.github.io

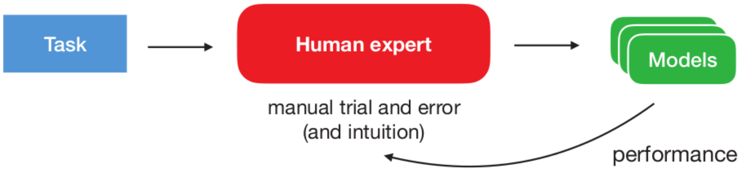
The Machine Learning Process

- Building an ML model is an iterative, complex, and time-consuming process.
- It can take a lot of trial and error.



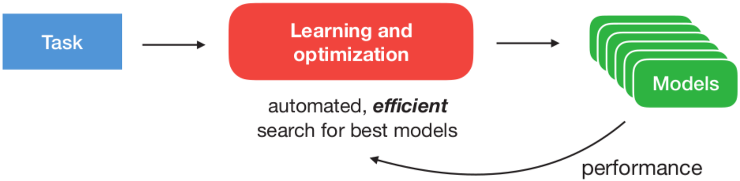
[Elshawi et al., Automated Machine Learning: State-of-The-Art and Open Challenges, 2019]

Automated vs. Manual Machine Learning



Automated vs. Manual Machine Learning

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

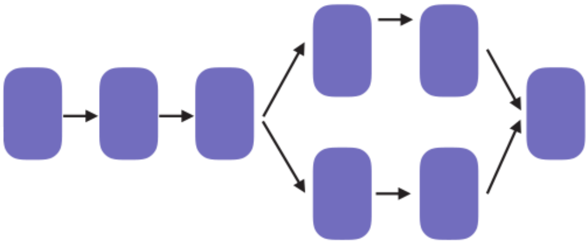


[Joaquin Vanschoren, Automatic Machine Learning - A Tutorial]


Search space design
Architecture search strategy
arch
score
Performance estimation strategy

AutoML Subproblems - Neural Architecture Search

- Represent and search all pipelines or neural nets, e.g., neural layers, interconnections, etc.



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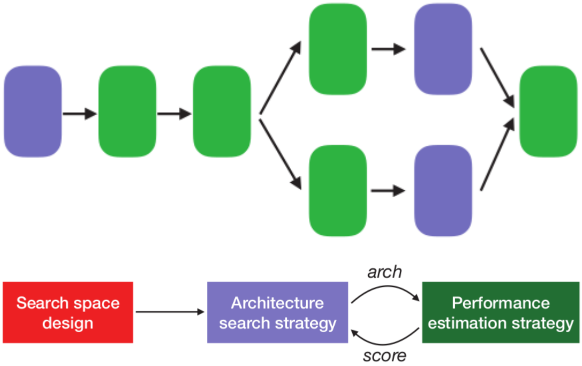
AutoML Subproblems - Hyperparameter Optimization

- Which hyperparameters are important? How to optimize them?



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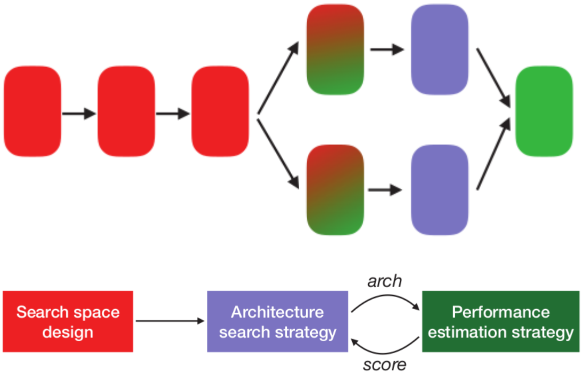
AutoML Subproblems - Meta-learning

- How can we transfer experience from previous tasks?
- Don't start from scratch (search space is too large).



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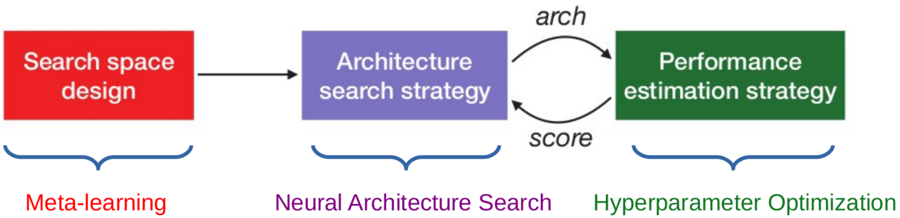
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Meta-learning
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Hyperparameter Optimization

Hyper-Parameter Optimization (HPO)

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- `A` denotes an ML algorithms with `m` hyperparameters.

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- $\mathtt{J}(\theta, \mathbf{X}_{\mathtt{train}}, \mathbf{X}_{\mathtt{valid}})$ is the loss of the ML model created by θ, trained on $\mathbf{X}_{\mathtt{train}}$, and validated on $\mathbf{X}_{\mathtt{valid}}$.
- Find the configuration that minimizes the expected loss on a dataset $\mathbf{X}_{\mathtt{train}}$:
  $\theta^* = \arg\min_{\theta \in \boldsymbol{\Lambda}} \mathbb{E}_{(\mathbf{X}_{\mathtt{train}}, \mathbf{X}_{\mathtt{valid}}) \sim \mathbf{X}} \mathtt{J}(\theta, \mathbf{X}_{\mathtt{train}}, \mathbf{X}_{\mathtt{valid}})$

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- Conditional
  - E.g., convolution kernel size, if convolution layer is selected

Hyper-Parameter Optimization

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- Multi-fidelity optimization

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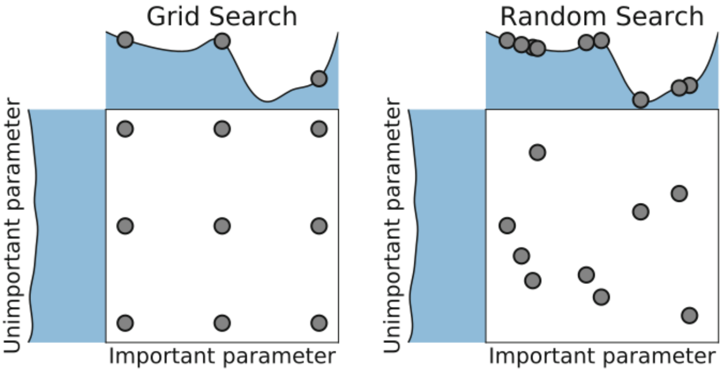
Black-box Optimization - Grid and Random Search



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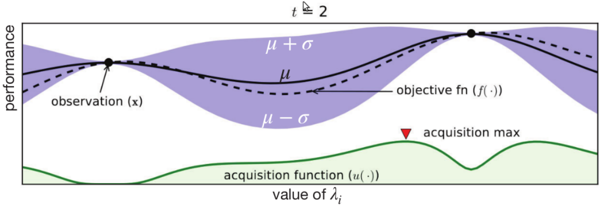
  - Combinations of different members (so-called crossover)
- E.g., genetic algorithms, evolutionary algorithms, particle swarm optimization

Black-box Optimization - Bayesian Optimization (1/3)

- Start with a few (random) hyperparameter configurations.



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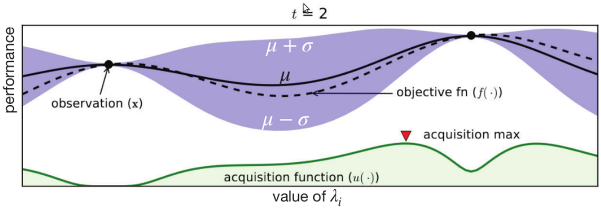

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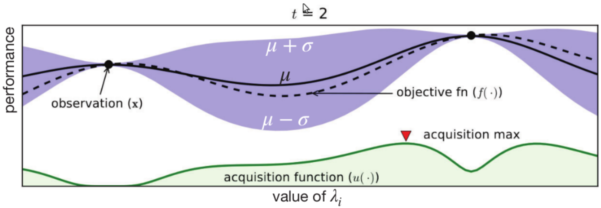

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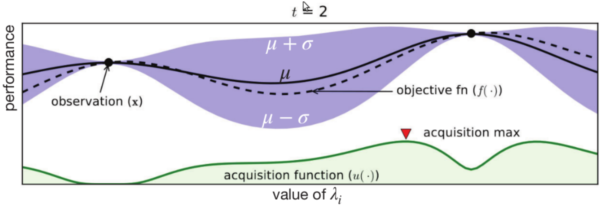
- Sample for the best configuration under that function.



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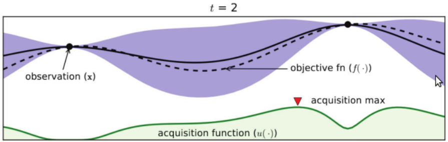

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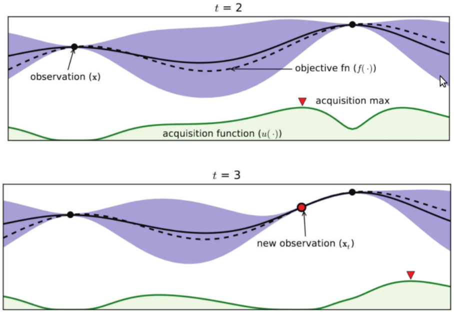

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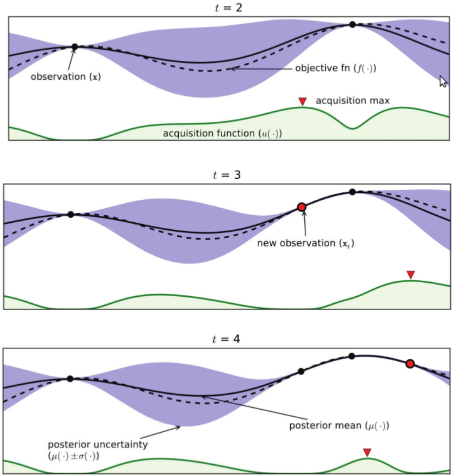

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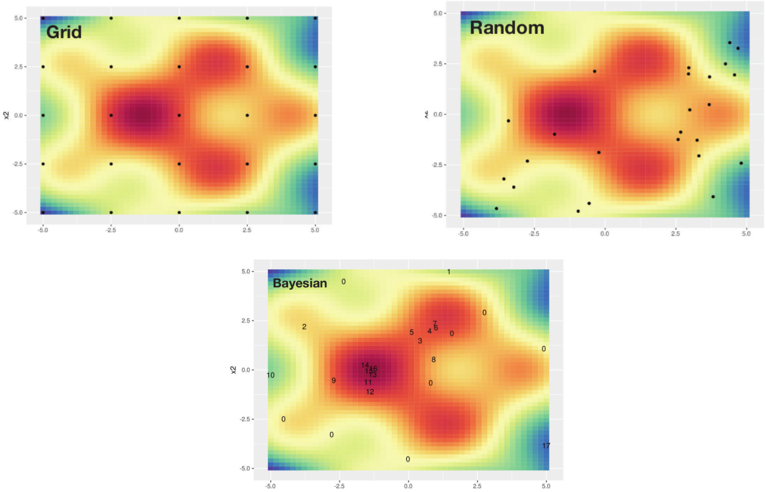
Black-box Optimization - Bayesian Optimization (3/3)



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Hyper-Parameter Optimization

- Black-box optimization
  - Grid search
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- These approximations introduce a tradeoff between optimization performance and runtime.

Multi-fidelity Optimization - Modeling Learning Curves

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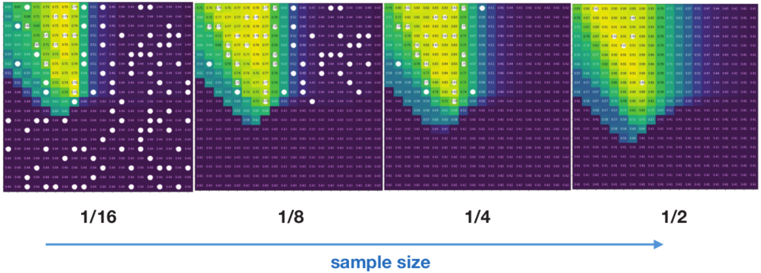
- Models learning curves during hyper-parameter optimization.
- Decides whether to allocate more resources or to stop the training procedure for a particular configuration.
- The learning process is terminated if the performance of the predicted configuration is less than the performance of the best model trained so far in the optimization process.

Multi-fidelity Optimization - Bandit-Based

- Successive halving algorithm (SHA)
- HyperBand

Multi-fidelity Optimization - SHA (1/4)

- Train on small subsets, infer which regions may be interesting to evaluate in more depth.



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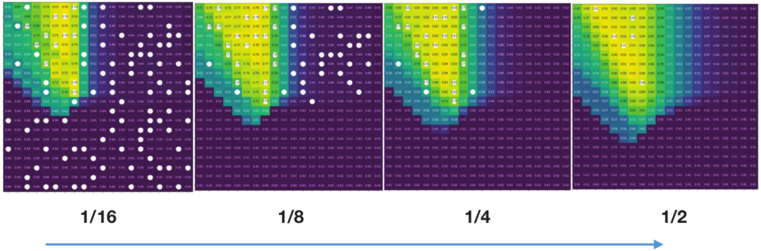

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Multi-fidelity Optimization - SHA (1/4)

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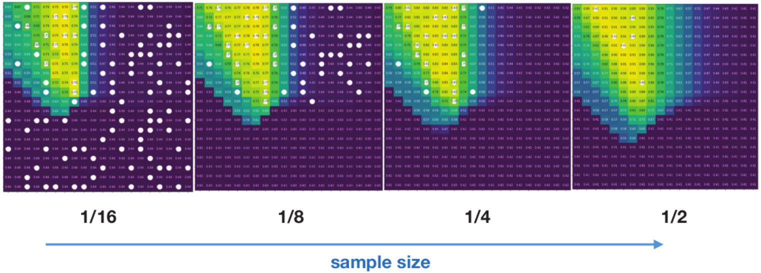
- E.g., retrain the 50% best candidates on twice the data.



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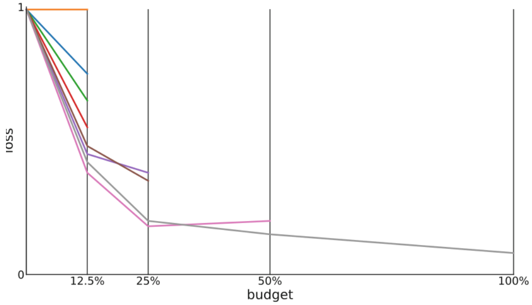
Multi-fidelity Optimization - SHA (2/4)

- Successive halving for eight algorithms/configurations.
- After evaluating all algorithms on 1/8 of the total budget, half of them are dropped and the budget given to the remaining algorithms is doubled.



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Multi-fidelity Optimization - SHA (3/4)

<u>SUCCESSIVEHALVING</u> (Finite horizon)

input: Budget B, and n arms where $\ell_{i,k}$ denotes the kth loss from the ith arm, maximum size R, $\eta \geq 2$ ($\eta = 3$ by default).

Initialize: $S_0 = [n]$, $s = \min\{t \in \mathbb{N} : nR(t+1)\eta^{-t} \leq B, t \leq \log_\eta(\min\{R, n\})\}$.

For $k = 0, 1, \ldots, s$

Set $n_k = \lfloor n\eta^{-k} \rfloor$, $r_k = \lfloor R\eta^{k-s} \rfloor$

Pull each arm in S_k for r_k times.

Keep the best $\lfloor n\eta^{-(k+1)} \rfloor$ arms in terms of the r_kth observed loss as S_{k+1}.

Output : $\hat{\imath}, \ell_{\hat{\imath},R}$ where $\hat{\imath} = \arg\min_{i \in S_{s+1}} \ell_{i,R}$

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- Assigning too large a budget can result in running poor configurations too long and thereby wasting resources.

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- Then it calls SHA on each set of random configurations.

Multi-fidelity Optimization - HyperBand (2/2)

Algorithm 1: HYPERBAND algorithm for hyperparameter optimization.

input : R, η (default $\eta = 3$)
initialization : $s_{\max} = \lfloor \log_\eta(R) \rfloor$, $B = (s_{\max} + 1)R$

for $s \in \{s_{\max}, s_{\max} - 1, \ldots, 0\}$ **do**
    $n = \lceil \frac{B}{R} \frac{\eta^s}{(s+1)} \rceil, \qquad r = R\eta^{-s}$
    `// begin SuccessiveHalving with` (n, r) `inner loop`
    $T =$ `get_hyperparameter_configuration`(n)
    for $i \in \{0, \ldots, s\}$ **do**
        $n_i = \lfloor n\eta^{-i} \rfloor$
        $r_i = r\eta^i$
        $L = \{$`run_then_return_val_loss`$(t, r_i) : t \in T\}$
        $T =$ `top_k`$(T, L, \lfloor n_i/\eta \rfloor)$
    end
end
return *Configuration with the smallest intermediate loss seen so far.*

- The inner loop invokes SHA for fixed values of `n` and `r`.
- The outer loop iterates over different values of `n` and `r`.

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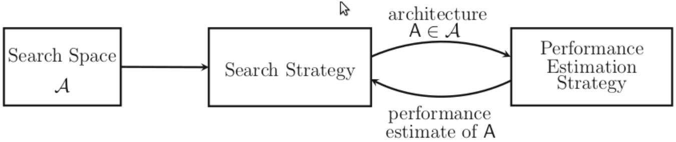

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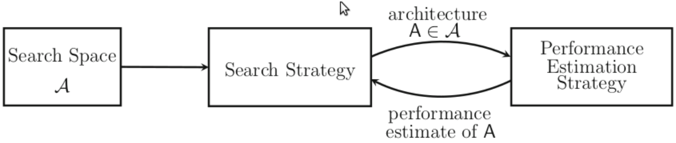

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Neural Architecture Search

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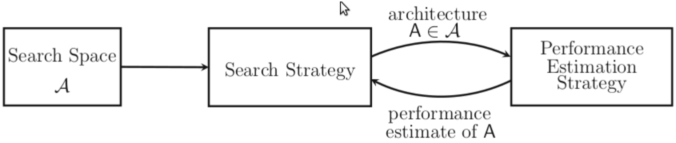
- Performance estimation: to perform a standard training and validation of the architecture on data.



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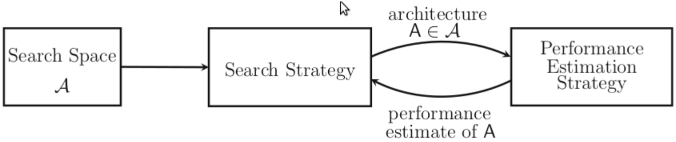
Search Space



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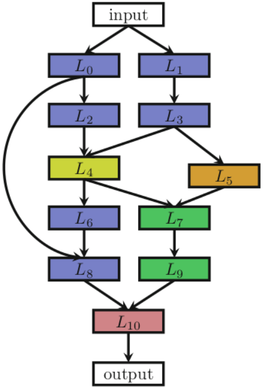
  - The type of operation every layer can execute, e.g., pooling, conv.
  - Hyperparameters associated with the operation, e.g., number of filters, kernel size and strides for a convolutional layer.

Multi-Branch Networks

- The input of layer i: a function $g_i(L_{i-1}^{out}, \cdots, L_0^{out})$ of previous layer outputs.



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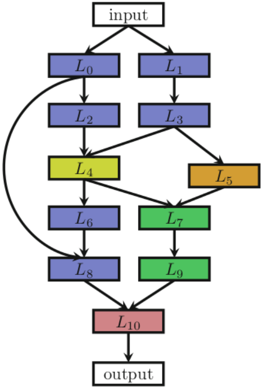

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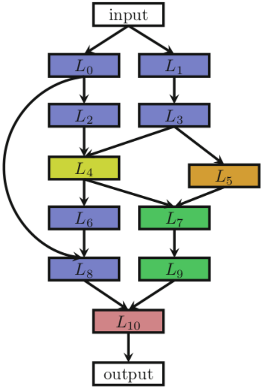

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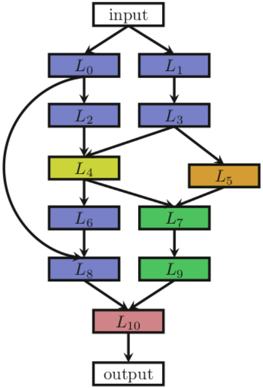

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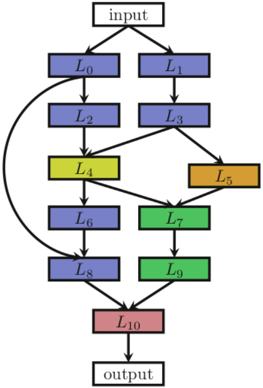
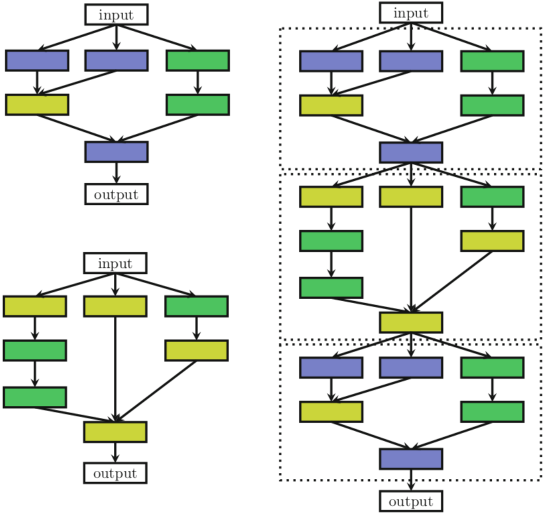
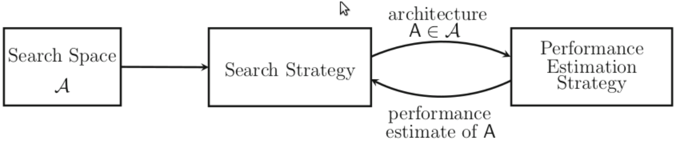


Repeated Motifs

- Normal cell: preservers the dimensionality of the input.
- Reduction cell: reduces the spatial dimension.



Search Strategy



Search Strategy

- Random search
- Reinforcement learning
- Gradient-based optimization
- Bayesian optimization
- Evolutionary methods

Random Search

- For each node in the DAG, determine what decisions must be made.

[Li et al., Random Search and Reproducibility for Neural Architecture Search, 2020]

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- Moving from node to node.

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- Evolutionary methods differ in how they sample parents, update populations, and generate offsprings.

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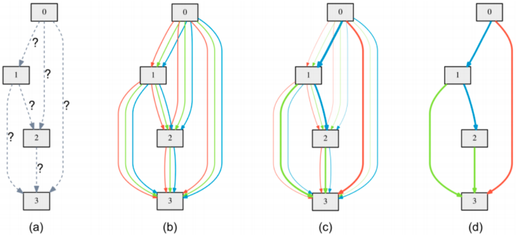

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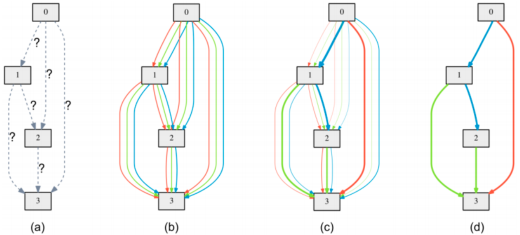

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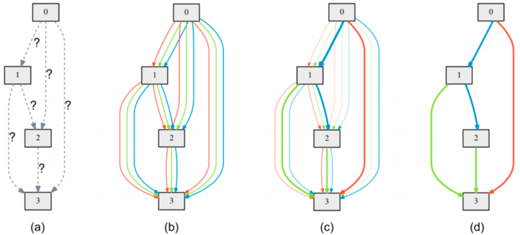
- We relax the categorical choice of a particular operation to a softmax over all possible operations.



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- The output is the architecture a^* with the largest value of $f(a^*)$ among all those that were tried in the previous rounds.

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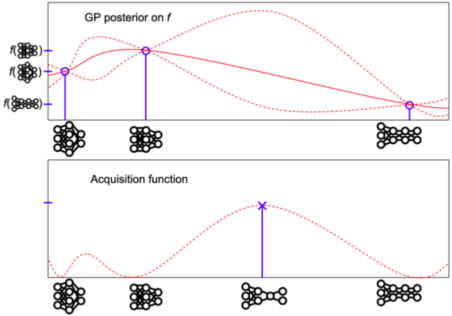
- The algorithm chooses $a_{i+1} = \arg\max_{a \in A} \max(0, E[f(a) - f^*]) = \arg\max_{a \in A} E[f(a)]$.
- f^* is the best accuracy observed so far.

Bayesian Optimization (3/3)

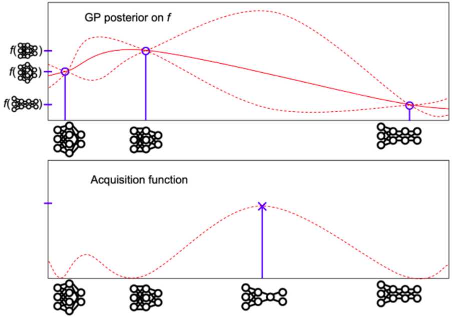
- The top graph: three evaluations of `f` (blue circles), an estimate of `f` (solid red line), and confidence intervals (dotted red lines).



[https://medium.com/abacus-ai/an-introduction-to-bayesian-optimization-for-neural-architecture-search-d324830ec781]

Bayesian Optimization (3/3)

- The top graph: three evaluations of `f` (blue circles), an estimate of `f` (solid red line), and confidence intervals (dotted red lines).
- The bottom graph: the expected improvement value for each architecture. The architecture with the largest expected improvement is chosen (blue `x`).



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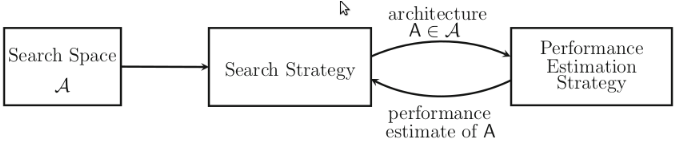
Performance Estimation



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- The simplest way of doing this is to train A on training data and evaluate its performance on validation data.
- However, training each architecture to be evaluated from scratch frequently yields computational demands in the order of thousands of GPU days for NAS.

Reduce the Computational Burden

- Low-fidelity approximation
- Learning curve extrapolation
- One-shot architecture

Meta-Learning

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- Then, learning from this experience (meta-data), to learn new tasks much faster than otherwise possible.

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- Learning from model evaluation
- Learning from prior models

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- The selection of meta-features is highly dependent on the application.

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- The similarity between two tasks is the distance between the feature vectors.

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- Building a meta-model $\mathtt{L}$ to learn the relationships between meta-features of prior tasks $\mathtt{t_j}$.
- For a new task $\mathtt{t_{new}}$, the meta-model $\mathtt{L}$ recommends the best configurations.

Learning from Prior Model Evaluation

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- Three different ways:
  1. Relative landmarks
  2. Surrogate models
  3. Warm-started multitask learning

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Learning from Prior Model Evaluation (2/3)

- Relative landmarks measure the performance difference between two model configurations on the same task
- Two tasks $\mathtt{t_{new}}$ and $\mathtt{t_j}$ are considered similar, if their relative landmarks performance of the considered configurations are also similar.
- Once similar tasks have been identified, a meta-learner can be trained on the evaluations $\mathtt{P_{i,j}}$ and $\mathtt{P_{i,new}}$ to recommend new configurations for task $\mathtt{t_{new}}$.

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- For a particular task $\mathtt{t_j}$, if the surrogate model can predict accurate configuration for a new task $\mathtt{t_{new}}$, then tasks $\mathtt{t_{new}}$ and $\mathtt{t_j}$ are considered similar.

Learning from Prior Models

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- Transfer learning usually works well when the new task to be learned is similar to the prior tasks.

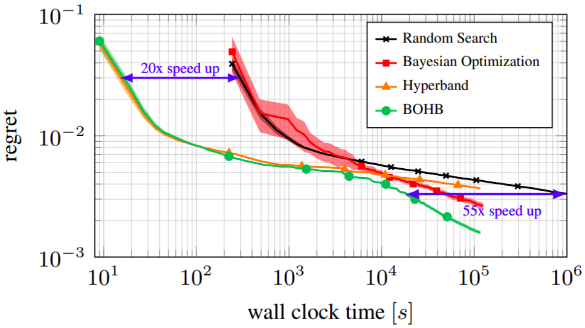
BOHB: Robust and Efficient Hyperparameter Optimization at Scale

BOHB: Bayesian Optimization and Hyperband

- Bayesian optimization (BO): for choosing the configuration to evaluate
- Hyperband (HB): for deciding how to allocate budgets

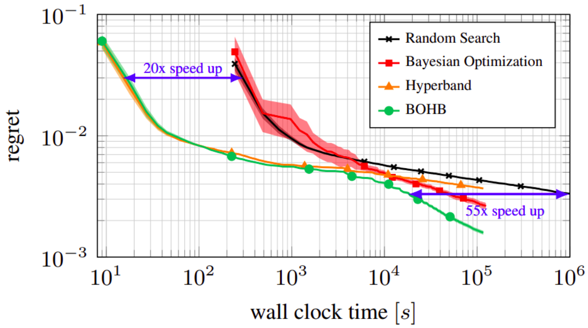
Bayesian Optimization vs. Random Search

- BO advantage: much improved final performance



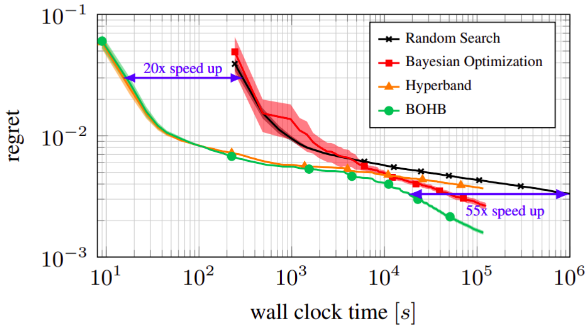
Hyperband vs. Random Search

- HB advantage: much improved anytime performance



Combining Bayesian Optimization and Hyperband

- Best of both worlds: strong anytime and final performance



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- Once the desired number of configurations for the iteration is reached, the SHA procedure is carried out using these configurations.

A System for Massively Parallel Hyperparameter Tuning

SHA

- SHA allocates a small budget to each configuration, evaluate all configurations and keep the top $\frac{1}{\rho}$.

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- SHA requires the number of configurations, a min and max resource, a reduction factor, and a minimum early-stopping rate.

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- If no promotions are possible, ASHA simply adds a configuration to the base rung, so that more configurations can be promoted to the upper rungs.
- Given its asynchronous nature it does not require the user to pre-specify the number of configurations to evaluate, but it otherwise requires the same inputs as SHA.

DARTS: Differentiable Architecture Search

Differentiable ARchiTecture Search (DARTS)

- Instead of searching over a discrete set of candidate architectures, we relax the search space to be continuous.
- The architecture can be optimized with respect to its validation set performance by gradient descent.

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- Each node $\mathtt{x}^{(\mathtt{i})}$ is a latent representation (e.g. a feature map in CNNs).
- Each directed edge $(\mathtt{i}, \mathtt{j})$ is associated with some operation $\mathtt{o}^{(\mathtt{i},\mathtt{j})}$ that transforms $\mathtt{x}^{(\mathtt{i})}$.
- Each intermediate node is computed based on all of its predecessors: $\mathtt{x}^{(\mathtt{j})} = \sum_{\mathtt{i}<\mathtt{j}} \mathtt{o}^{(\mathtt{i},\mathtt{j})}(\mathtt{x}^{\mathtt{i}})$

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$\overline{\mathtt{o}}^{(\mathtt{i},\mathtt{j})}(\mathtt{x}) = \sum_{\mathtt{o}\in\mathcal{O}} \frac{\exp(\alpha_{\mathtt{o}}^{(\mathtt{i},\mathtt{j})})}{\sum_{\mathtt{o}'\in\mathcal{O}} \exp(\alpha_{\mathtt{o}'}^{(\mathtt{i},\mathtt{j})})} \mathtt{o}(\mathtt{x})$

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- At the end of search, a discrete architecture can be obtained by replacing each mixed operation $\overline{\mathtt{o}}^{(\mathtt{i},\mathtt{j})}$ with the most likely operation, i.e., $\mathtt{o}^{(\mathtt{i},\mathtt{j})} = \arg\max_{\mathtt{o}\in\mathcal{O}} \alpha_{\mathtt{o}}^{(\mathtt{i},\mathtt{j})}$.

Summary

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- Hyperparameter optimization
  - Black-box optimization
  - Multi-fidelity optimization
- Nural architecture search
  - Search space
  - Search strategy
  - Performance estimation
- Meta-learning
  - Learning from task properties
  - Learning from prior model evaluation
  - Learning from prior models

Reference

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Questions?