Module 5

Evi Gogoulou, Shahbaz Khader, Akhila Rao

Automated Machine Learning: State-of-The-Art and Open Challenges

Radwa Elshawi Mohamed Maher Sherif Sakr

Problem definition

- CASH Problem : Combined Algorithm Selection and Hyper-parameter tuning

$$A^{(i)^*} \in \underset{A \,\epsilon\, \mathbf{A}}{argmin}\ L(A^{(i)}, D_{train}, D_{validation})$$

- Goal: Select an ML algorithm that can achieve optimal performance in both the training and validation set, given a *specific time budget constraint*.

Meta-Learning

- Warm starting of the optimization algorithm by leveraging previous learning experiences.
- Learning based on task properties:
  - Use constructed meta-features to compute the similarity between two datasets
  - Build a meta-model that learns the statistical properties of the previous dataset
- Learning from previous model evaluations:
  - Train a meta-learner on previous evaluations of the ML model (parameters θ_i , task t_i) to predict new parameters Θ^* new for a new task t^*
- Learning from already pretrained models:
  - Transfer Learning: utilize pretrained models, trained on a task t_i , for training on a new task t_j given certain similarity between t_i and t_j

Neural Architecture Search for Deep Learning

- Technique for automatic design of deep Artificial Neural Networks
- Random Search:Randomly sample neural architectures from a bounded search space
- Reinforcement Learning: An agent explores the finite search space of architectures with the goal of maximizing the performance on the given task
- Gradient-based optimization: Explore the continuous search space with the help of gradient descent
- Evolutionary Methods: They are based on genetic algorithms or hierarchical evolution
- Bayesian optimization: They rely on Gaussian processes or tree-based models

Hyperparameter Optimization (1)

- Black-Box optimization: The analytical form of the objective function is not known, only the results of evaluating this function at different points can be used.
- Grid Search \ Random Search:
    - Easily parallelizable methods
    - Given a computational budget, random search is better
- Bayesian Optimization: Suitable for computationally expensive objective functions
- Simulated Annealing: Update each hyperparameter value based on the neighbourhood states
- Genetic Algorithms: Apply genetic operations to a population of hyperparameter configurations

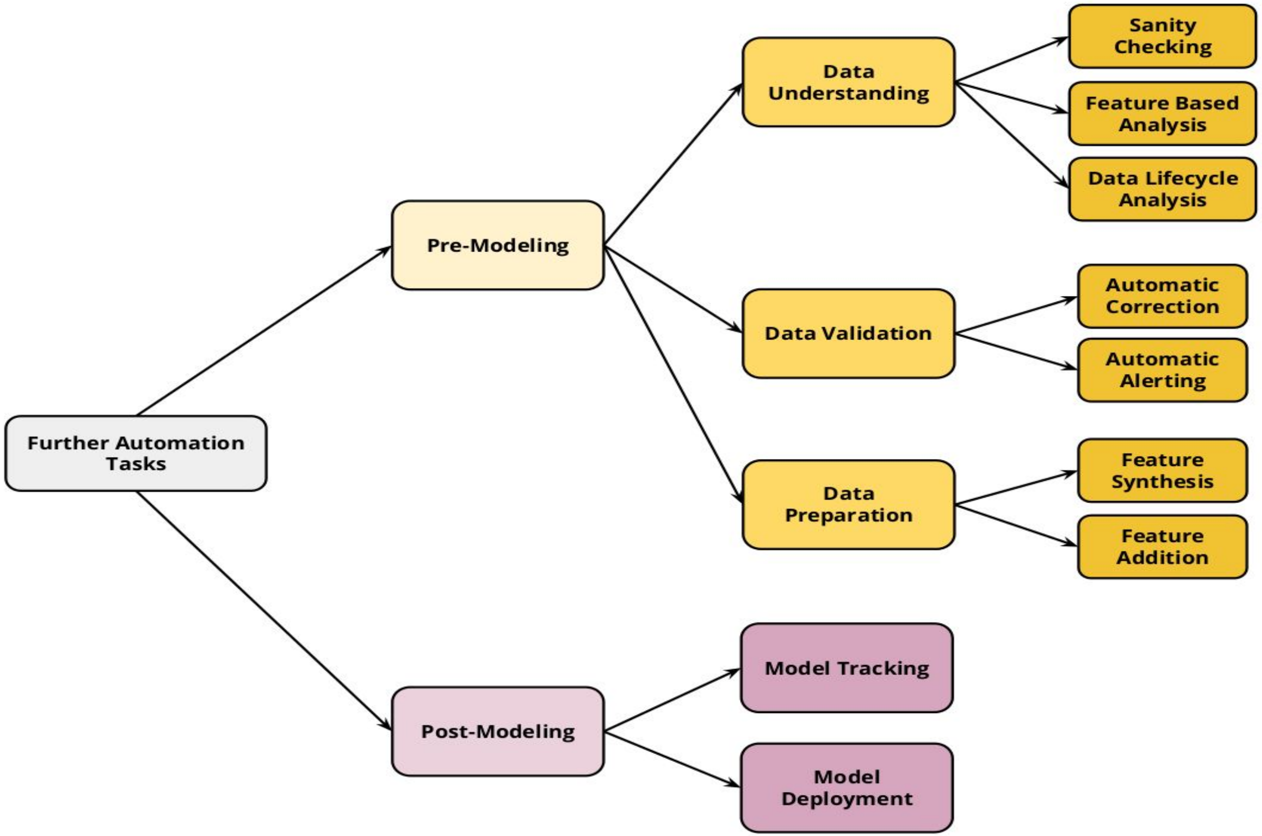
Hyperparameter Optimization (2)

- <u>Multi-fidelity optimization:</u> Use a small part of the dataset to evaluate the objective function (low-fidelity evaluation)
    - Use many low-fidelity evaluation instead of one high-fidelity evaluation
    - Trade-off between computational cost and optimization performance
- Modeling learning curves: Uses the progression of the learning curve as the stopping criterion for the hyperparameter optimization
- Successive halving: multi-fidelity method which keeps only the best half of the tested configurations at each step
- HyperBand: multi-fidelity method that applies Successive halving on randomly sampled configurations

Tools and Frameworks

- Centralized Frameworks:
  - designed to run on a single machine
  - suitable for handling small to medium datasets
- Distributed Frameworks:
  - Utilize multi-node systems for solving the CASH probrem for bigger datasets
- Cloud-based Frameworks:
  - Utilize the computational power of cloud-based environments
  - Typically require minimal user experience
  - Compatible with other services in the same cloud ecosystem
- Neural Network Automation Frameworks:
  - find neural network architectures that are competitive with architectures designed by human expert

Other automation aspects



Summary

- Good overview of all available methods and tools for automatizing the ML pipeline
- It would be probably insightful to analyse all the presented methods from the perspective of the budget constraint
- Expand the survey to include AutoML methods for massive neural architectures

Hyperparameter Optimization

- Machine learning algorithms can be very sensitive to hyperparameter settings. So choosing the right one is crucial.
- Hyperparameters
  - Learning rate
  - Regularization
  - Architecture
- Budget
  -

BOHB: Robust and Efficient Hyperparameter optimization at Scale

Stefan Falkner, Aaron Klein, Frank Hutter

PMLR 2018

Motivation

- Bayesian based methods for HPO are typically computationally infeasible.
- Random search based methods (such as Hyperband) are faster but do not converge to good solutions.

Contribution

- Create a best of both worlds approach called BOHB

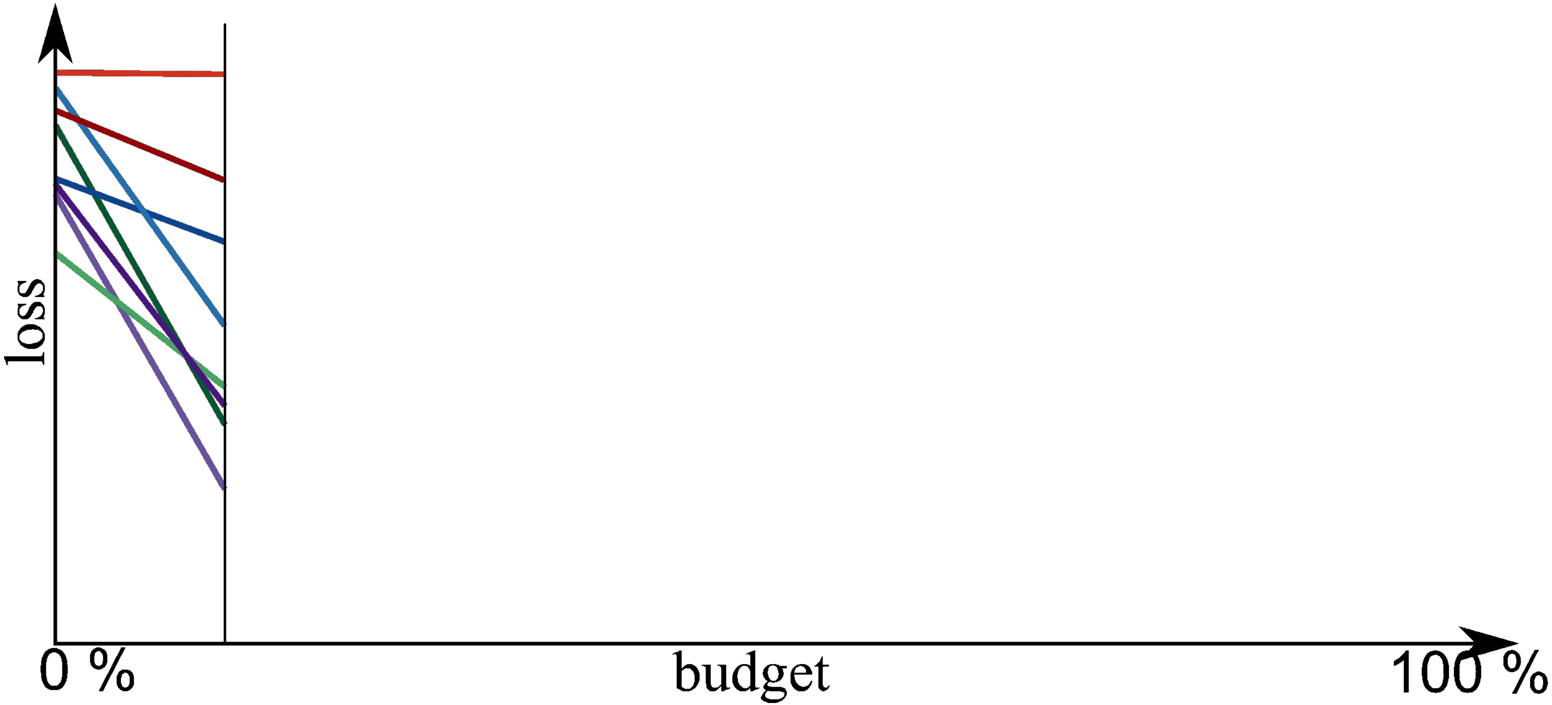
Bayesian Optimization (BO)

- Density over input configuration space is estimated to select new candidate configurations to evaluate.

Hyperband (HB)

- Cheap to evaluate approx. versions of objective function are defined given a budget. Higher the budget higher the quality of the estimate.
- Budget here can be the num. of iterations, num. of data points, num. of steps in MCMC algo., num. of trials in deep reinforcement learning etc.
- Invoke successive halving (SHA) to select and promote configurations.

Successive Halving (SHA)



- Distribute the budget over ‘n’ random initial configurations.
- Evaluate and promote the best half to the next rung with double the budget.
- Iterate till one remains.

BOHB

Algorithm 2: Pseudocode for sampling in BOHB

input : observations D, fraction of random runs ρ, percentile q, number of samples N_s, minimum number of points N_{min} to build a model, and bandwidth factor b_w

output : next configuration to evaluate

if *rand()* < ρ **then return** random configuration

$b = \arg\max\{D_b : |D_b| \geq N_{min} + 2\}$

if $b = \emptyset$ **then return** random configuration

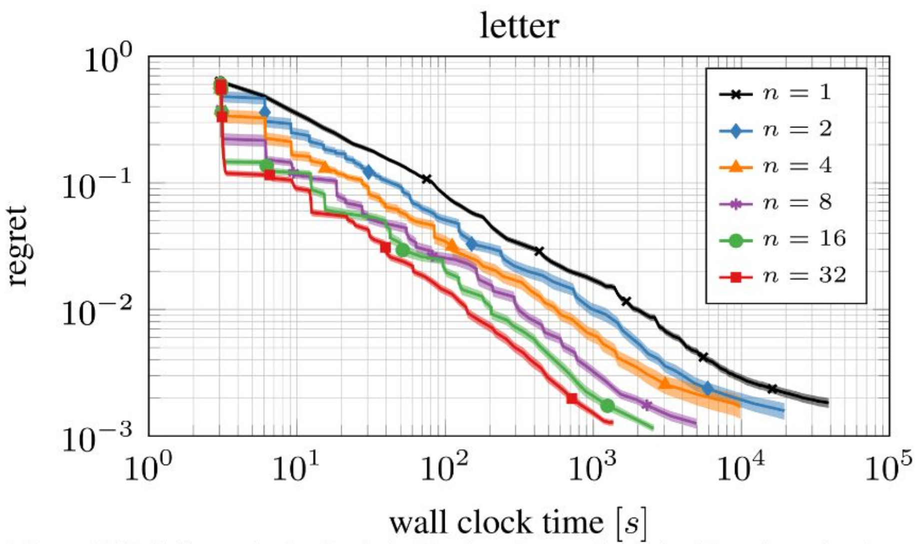
fit KDEs according to Eqs. (2) and (3)

draw N_s samples according to $l'(\boldsymbol{x})$ (see text)

return sample with highest ratio $l(\boldsymbol{x})/g(\boldsymbol{x})$

- BO does model based search for suitable configurations.
- HB selects the num. of configurations and assigns budget.
- Model is updated based on evaluated configurations.
- Iterate.

Parallel resources

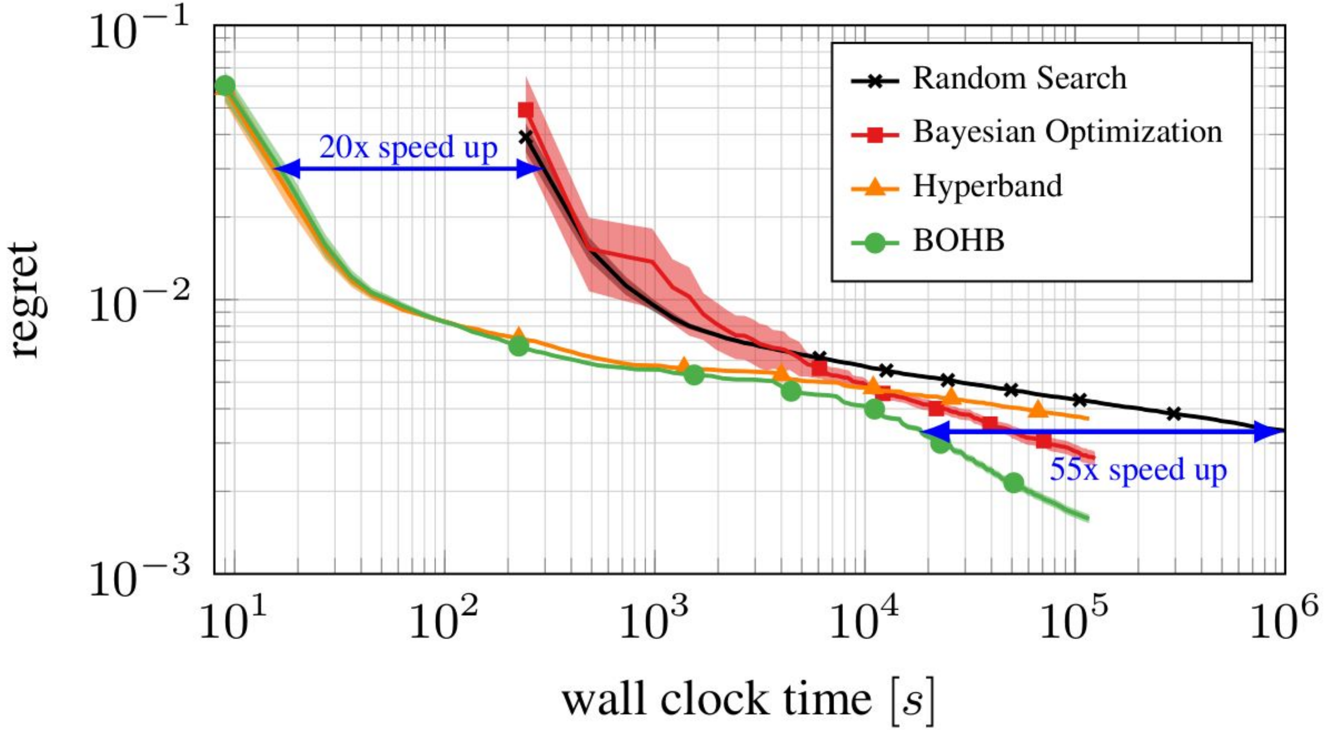


Performance of BOHB with different number of parallel workers for 128 iterations on the surrogate letter benchmark. The speedups are close to linear.

- In BOHB multiple configurations need to be evaluated independently at each iteration.
- This can be parallelized.

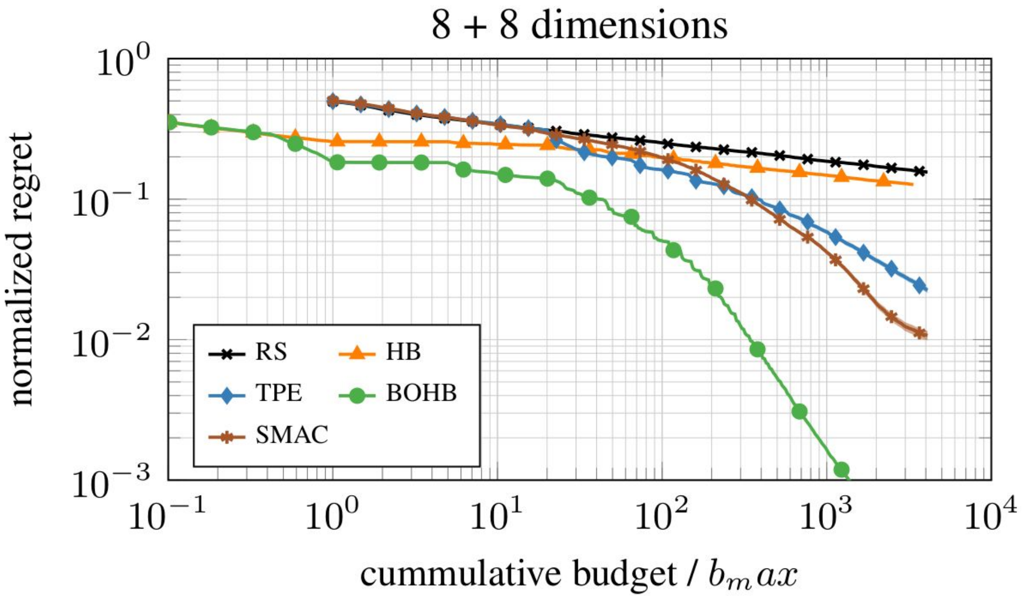
Evaluation over various scenarios

Best of both worlds: BOHB

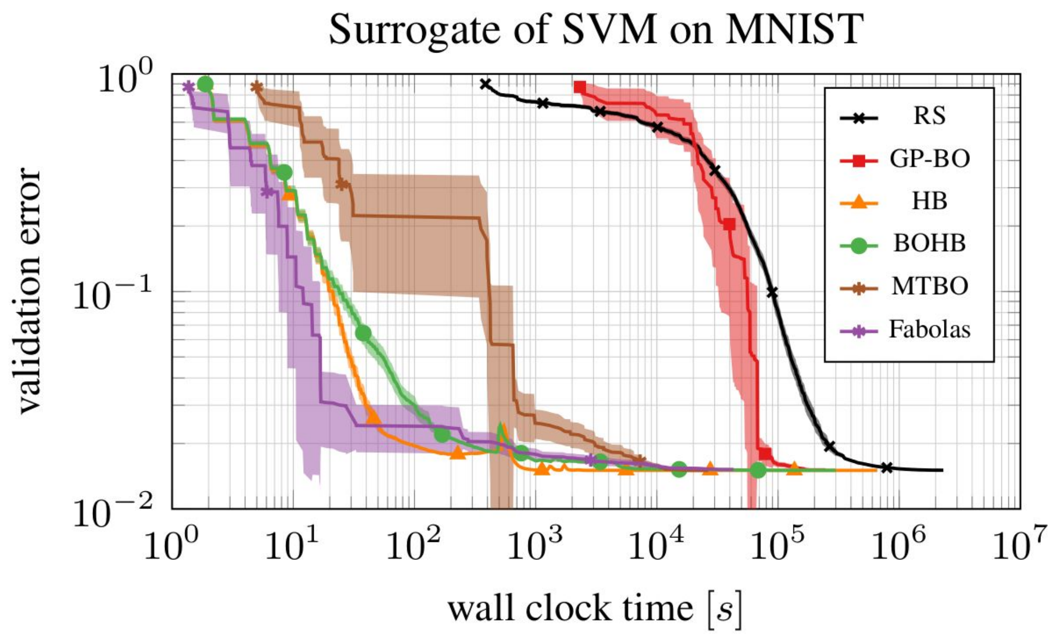


- Optimizing 6 hyperparameters of a neural network.
- Has strong anytime performance obtained from HB.
- Has strong final performance obtained from BO.

Stochastic Counting Ones

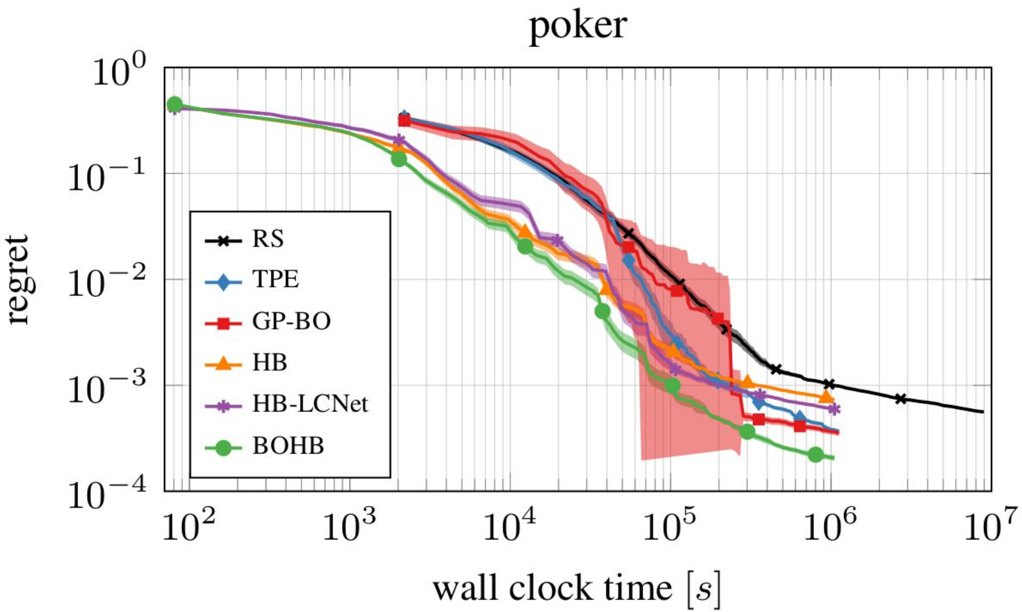


Support Vector Machines

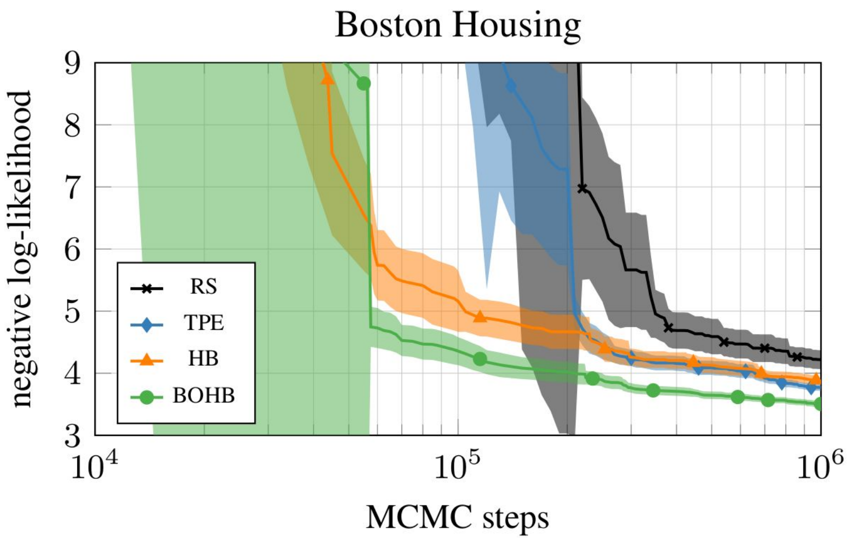


- Setup: Surrogate imitates optimization of SVM with RBF kernel
- Tunable hyperparameters (2)
- Budget: num. of training data points for HB, BOHB, full set for the others.
- Take away: GP-BO and RS are too slow. Fabolas, HB and BOHB find good configuration quickly with Fabolas having the fastest initial speedup.

Feed-forward Neural Networks



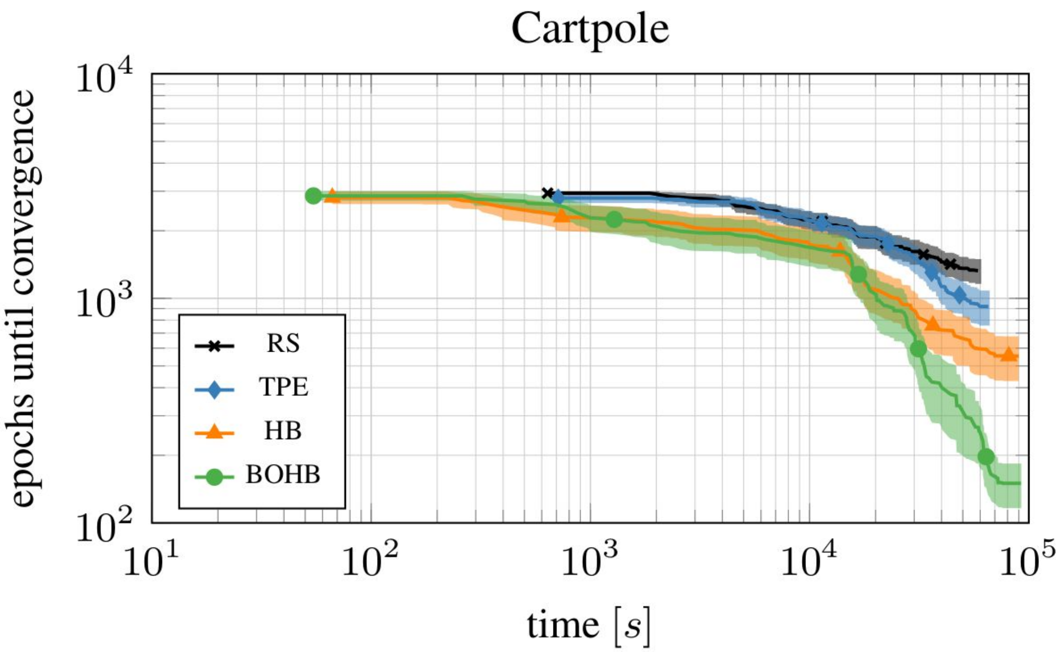
Bayesian Neural Networks



- Setup: 2 layered fully connected Bayesian neural network trained with MCMC sampling.
- Tunable hyperparameters (4):
  - step length,
  - length of burn-in period,
  - num. of units in each layer,
  - decay parameter of momentum.
- Dataset: Boston housing
- Budget: 500-10000 MCMC steps

Take away: BOHB converged faster than both HB and TPE (BO) and even found a better configuration than the baselines.

Reinforcement Learning



- Setup: Proximal policy optimization to learn the cartpole swing-up task.
- Tunable hyperparameters (8)
- Budget: BOHB and HB 1-9 trials, others fixed 9 trials.
- Take away: BOHB starts same as HB but converged to better configurations. TPE did not have enough budget to find the same.

Convolutional Neural Networks

- Tunable hyperparameters: learning rate, momentum, weight decay, batch size.
- Budget: 22,66,200,600 epochs.
- 19 parallel workers
- Take away: BOHB is practically useful for resource constrained optimization.

Limitations

- Small budgets gives us cheap approximations of objective function.
- This assumes that relative ranking of configurations mostly hold even for small budgets.
- If this is not true and the approximation is too noisy then it will result in BHOB being slower than BO and worse than than even random search.
- To overcome this BHOB samples a fixed fraction (1/3) of configurations randomly. This avoids missing good configurations hiding among bad ones.

Summary

- BOHB combines good initial performance of HB and good convergence properties of BO.
- BO component helps guide the search and results in faster convergence
- HB component helps get a quick start through SHA and results in good initial speedup.
- Solution is robust , flexible, scalable gives strong anytime and final performance.
- Code has been made available.

A System for Massively Parallel Hyperparameter Tuning

Liam Li, Kevin Jamieson, Afshin Rostamizadeh, Ekaterina Gonina, Jonathan Ben-Tzur, Moritz Hardt, Benjamin Recht, Ameet Talwalkar

MLSys 2020

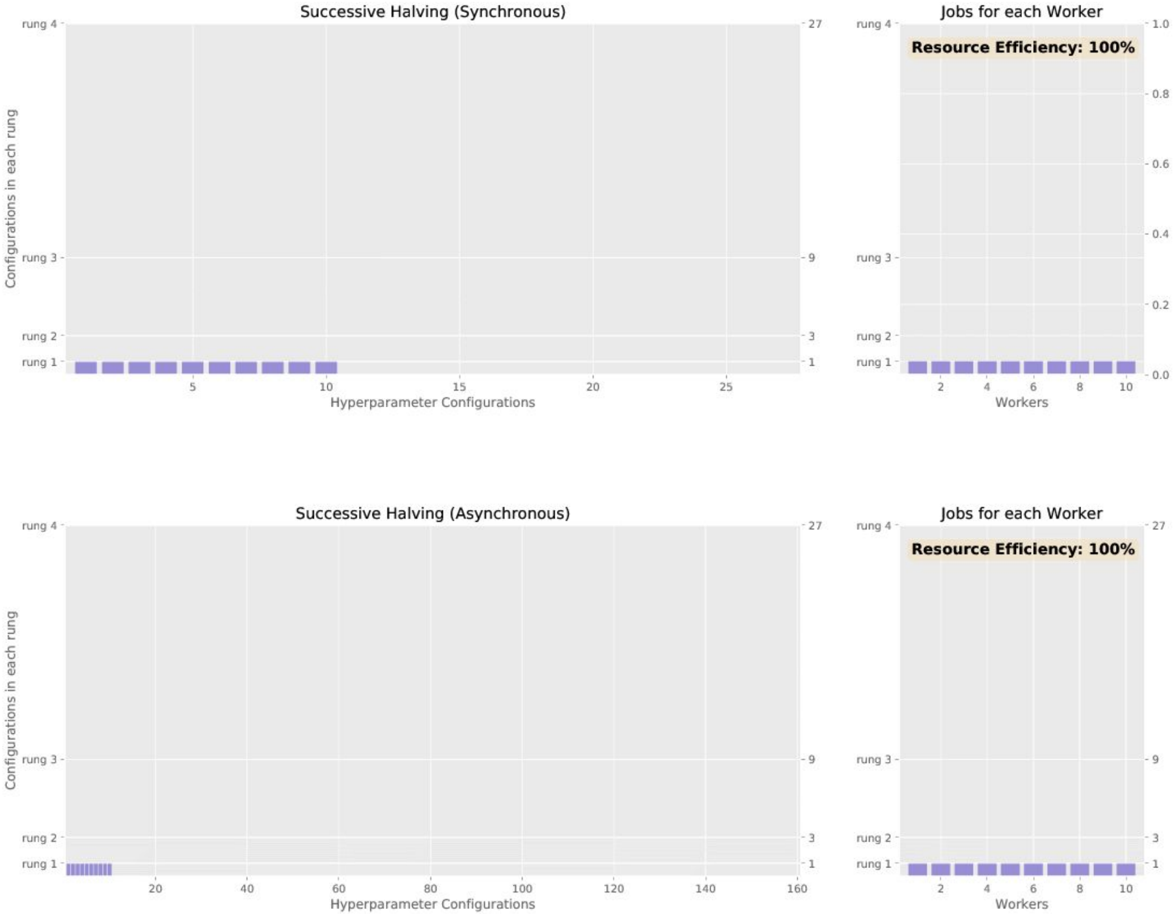
Motivation

- Usually, with increasingly large models, the available additional budget for HPO is low.
- Massive parallelization is the way to go.
- Adaptive search based methods are iterative and hard to parallelize.
- Grid and random search are trivial to parallelize but don’t scale well with increased num. of hyperparameters.
- Synchronous hyperparameter tuning methods struggle from stragglers.
- There is a need for production grade hyperparameter tuning systems.

Contribution

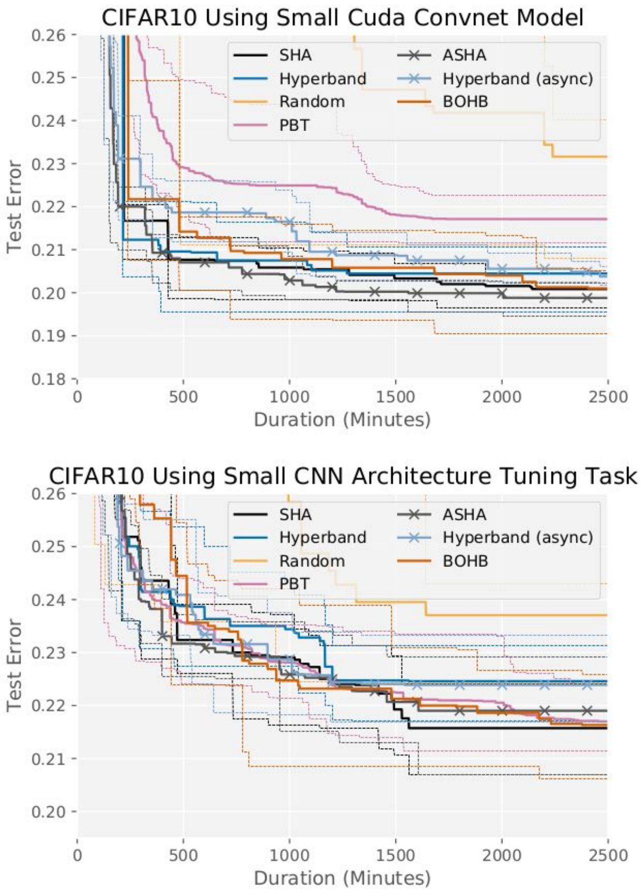
- Asynchronous SHA called ASHA.
- A method to parallelize ASHA.
- Deploy ASHA in a production grade system.

Async SHA: ASHA



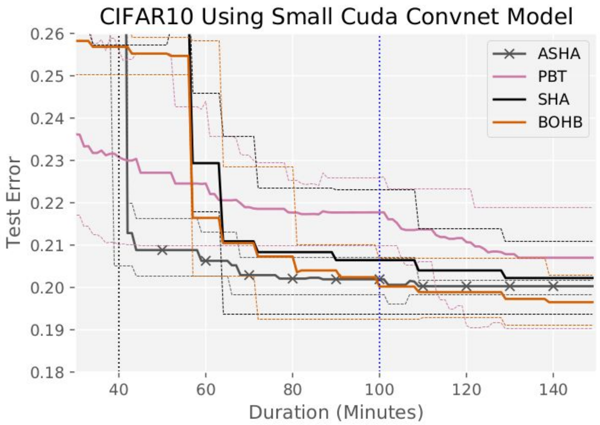
- When a worker finishes a job it requests a new one.
- We look at the rungs from top to bottom to see if there are configurations in the top 1/η of each rung.
- These are promoted to the next rung.
- If none, we assign the worker to add a configuration to the lowest rung to grow the width of the level so that more configurations can be promoted.

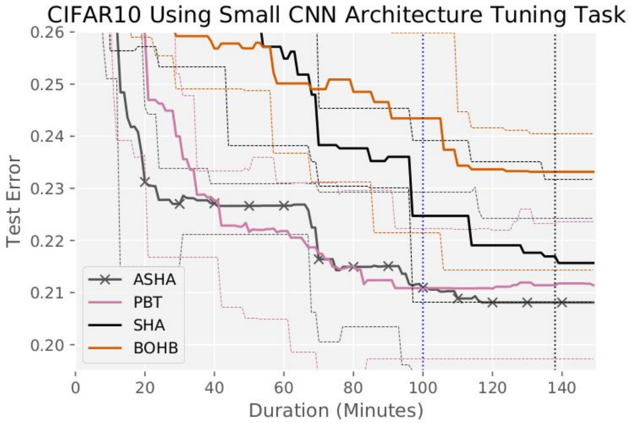
Single Machine Experiments



- PBT is the state-of-the-art evolutionary method that iteratively improves fitness of configurations.
- Benchmark 1:
  - SHA and ASHA do better than PBT.
- Benchmark 2:
  - SHA, ASHA and PBT do comparably.
- Both cases, ASHA does not degrade performance even though it is async.

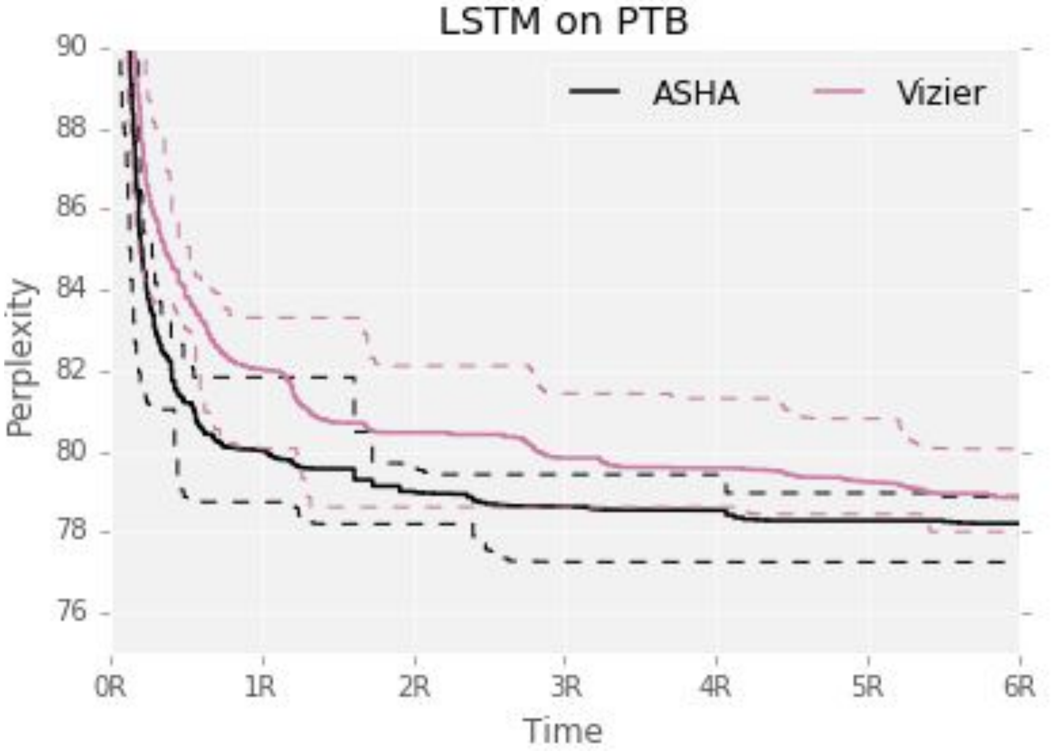
Distributed experiments





- 25 workers.
- Benchmark 1:
  - ASHA better than PBT, comparable to BOHB.
  - ASHA took 40 min to evaluate 1000 configurations and find a good one using 25 workers.
  - This is about the same time as needed to train for a single configuration on 1 worker.
  - In a serial setting this would take 400 min.
  - Increase in # workers by 25 led to only 10 X speedup due to relative simplicity of the task.
- Benchmark 2:
  - ASHA comparable to PBT, better than BOHB.
  - ASHA took 25 min while using 25 workers.
  - It took 700 min while using 1 worker.
  - Speedup in linear since this is a harder task that can leverage the additional workers.

Distributed Large-scale experiments



- 500 workers.
- Vizier is Google's internal hyperparameter optimizer.

Production grade ASHA

- Simplified user interface with same input as random search.
- Stopping criteria is a fixed number of configurations.
- Use Paleo predicted trade-off curves to choose number of GPUs per configuration for a given efficiency.
- A fair share scheduler that adaptively allocated resources over the lifetime of a job.
- Reproducible checkpoints and state saving for pause and restart feature.

Summary

- Making SHA async (ASHA) does not degrade its performance and allows for massive parallelization of HPO.
- Parallelized ASHA does comparable or better than PBT, SHA and BOHB.
- A production grade HPO system was developed with many contributions in the form of informed design decisions.

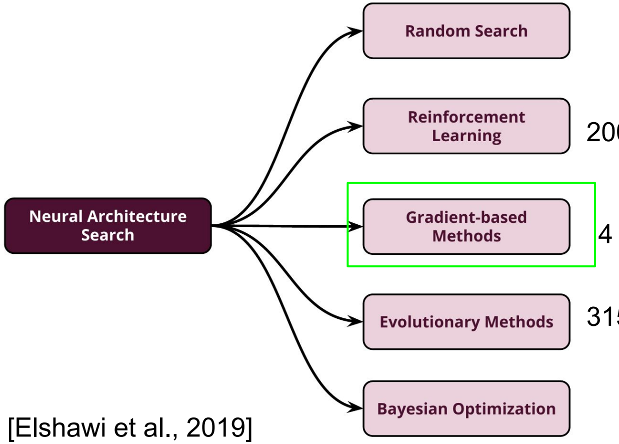
Network Architecture Search (NAS)

DARTS: DIFFERENTIABLE ARCHITECTURE SEARCH

Hanxiao Liu, Karen Simonyan, Yiming Yang

ICLR 2019

Motivation



2000 GPU days [Zoph et al., 2018]

4 GPU Days, DARTS

3150 GPU days [Real et al., 2018]

[Elshawi et al., 2019]

Main problem: large discrete search space

SOTA methods are gradient-free:

- Black-box search in a discrete non-differentiable space
- Significantly slower

Main contribution

A method for gradient-based search for network architecture:

- Main idea: relax the discrete set of candidate architecture to be a continuous space and apply gradient descent

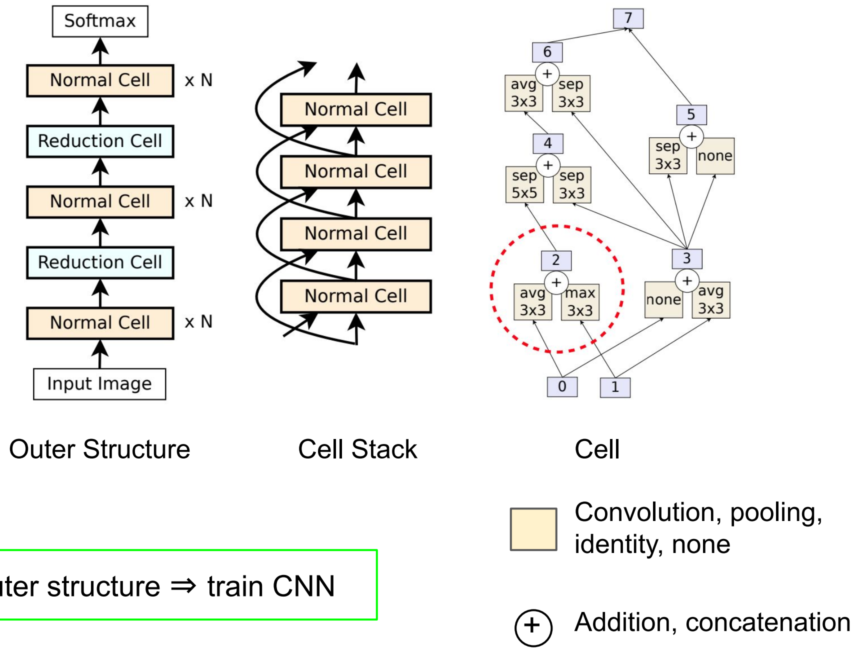
- Orders of magnitude gain in computation time due to the better efficiency of gradient-based optimization

- Generic enough for CNN and RNN

NASNet Search Space and the Cell [Zoph et al., 2018]

Steps:

1. Constrain all cells to have the same architecture
2. Design a small outer structure and search for a cell architecture on a smaller dataset (CIFAR-10)
3. Preserve the cell architecture and scale up to a larger outer structure
4. Train on a larger dataset (ImageNet) that we really want



Fix outer structure ⇒ search operations in a cell ⇒ scale up outer structure ⇒ train CNN

DARTS: Continuous Search Space

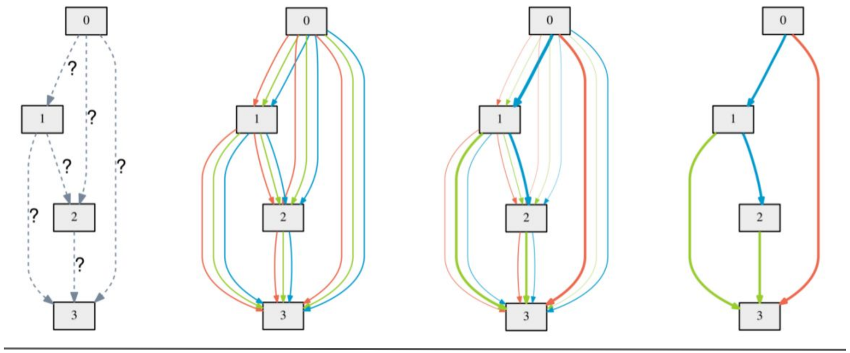
A cell is a DAG consisting of sequence of N nodes:

- Each node $x^{(i)}$ is an intermediate result (tensor)
- Each directed edge (i,j) is an operation (e.g. convolution)
- Two input nodes and a single output node

For each intermediate node j : $x^{(j)} = \sum_{i<j} o^{(i,j)}(x^{(i)})$

Output of the cell is obtained by reduction operation (addition / concatenation) to all intermediate nodes

N=4



Continuous relaxation and optimization:

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

$\mathcal{O}$ is the set of operations and dim $\alpha^{(i,j)}$= $|\mathcal{O}|$

CNN

$\mathcal{O}$:

3X3, 5X5 sep & dilated sep conv
3X3 max & avg pooling
Zero
N=7
Cell stack

RNN

$\mathcal{O}$:

Linear transformations
tanh, relu, sigmoid
Identity, Zero
N=12
Single cell

Architecture search :
Learn $\alpha = \{\alpha^{(i,j)}\}$ (set of continuous mixing weights) and $o^{(i,j)} = \mathrm{argmax}_{o \in \mathcal{O}} \ \alpha_o^{(i,j)}$

Bilevel Optimization

Joint learning of architecture α and network weights w.

Optimize for α^*

$$\min_{\alpha} \quad \mathcal{L}_{val}(w^*(\alpha), \alpha)$$
$$\text{s.t.} \quad w^*(\alpha) = \text{argmin}_w \ \mathcal{L}_{train}(w, \alpha)$$

Approximation:

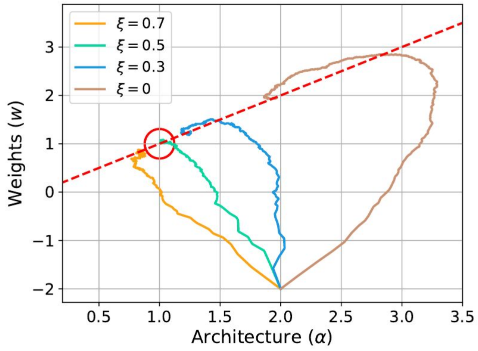
$$\nabla_\alpha \mathcal{L}_{val}(w^*(\alpha), \alpha)$$
$$\approx \nabla_\alpha \mathcal{L}_{val}(w - \xi \nabla_w \mathcal{L}_{train}(w, \alpha), \alpha)$$

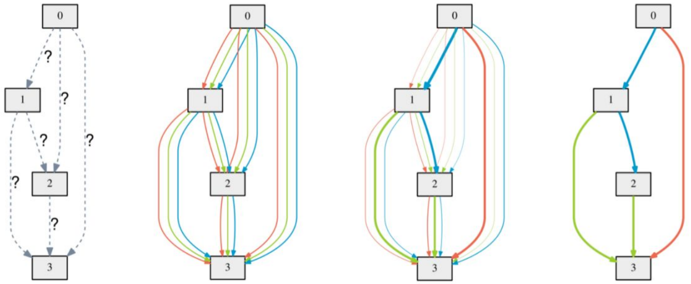
Final architecture selection:

$$o^{(i,j)} = \text{argmax}_{o \in \mathcal{O}} \ \alpha_o^{(i,j)}$$

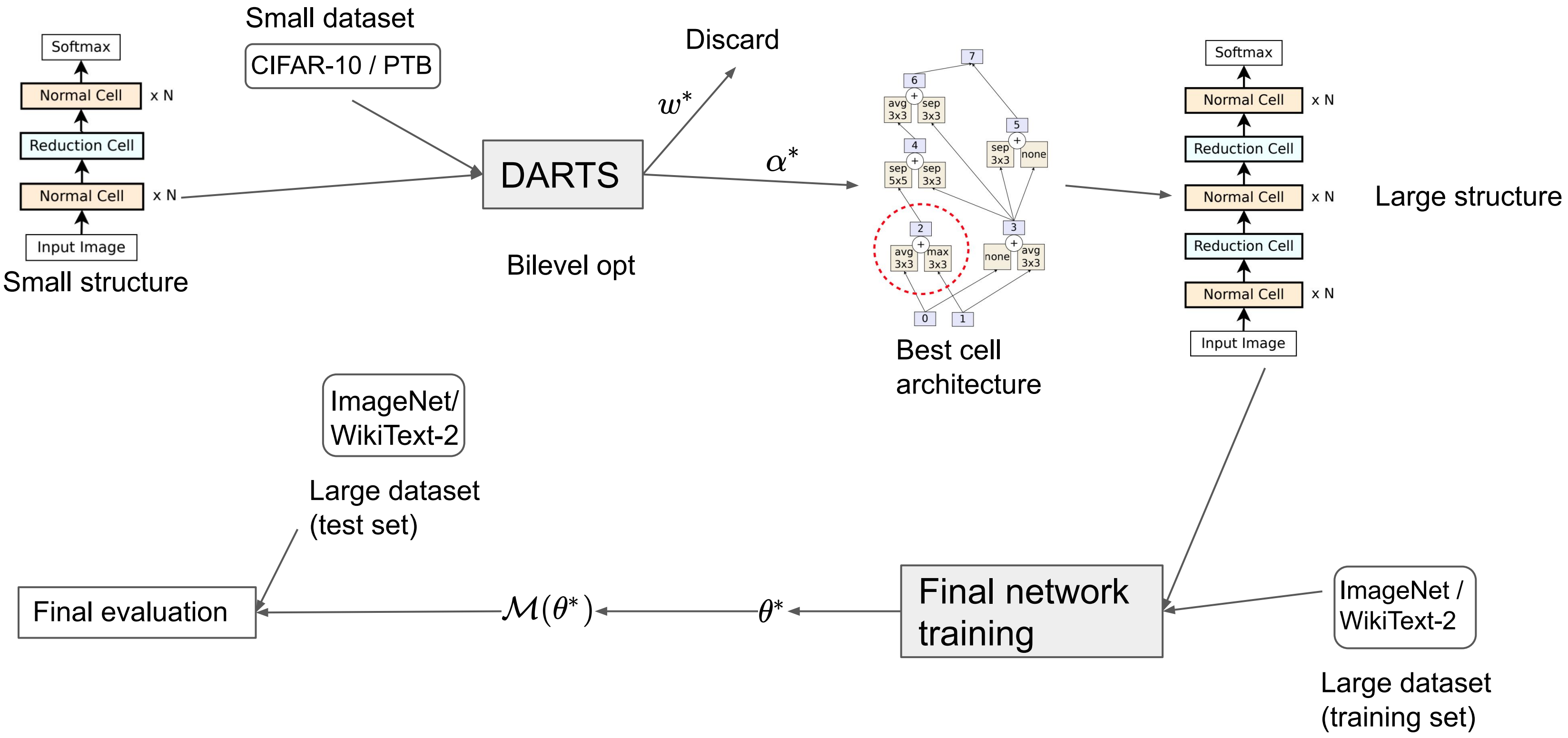
But, a node could be connected to too many predecessors!

DARTS employs pruning: retain only k strongest connections

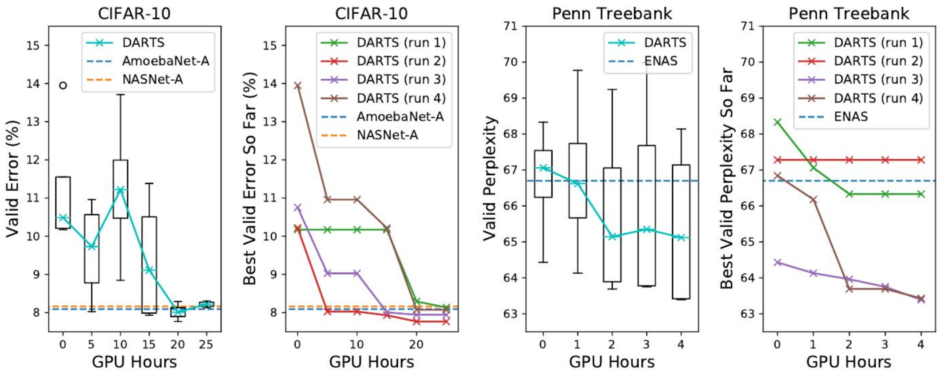


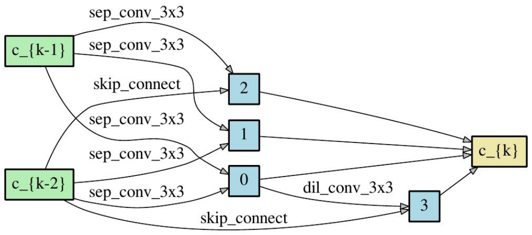


Experiment design

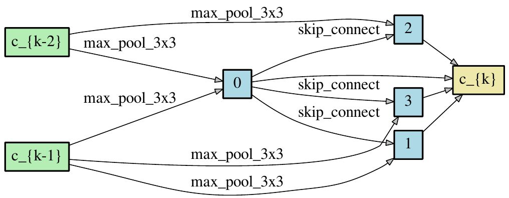


Learned Cells

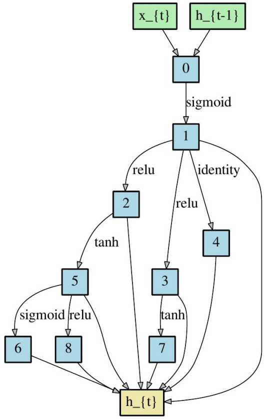




Normal cell (CIFAR-10)



Reduction cell (CIFAR-10)



Recurrent cell (PTB)

Note:

1. Exactly 2 incoming connections for CNN cells
2. Exactly 1 incoming node for RNN cells
3. The above are enforced through a pruning strategy

Comparison

Architecture	Test Error (%) top-1	Test Error (%) top-5	Params (M)	$+\times$ (M)	Search Cost (GPU days)	Search Method
Inception-v1 (Szegedy et al., 2015)	30.2	10.1	6.6	1448	–	manual
MobileNet (Howard et al., 2017)	29.4	10.5	4.2	569	–	manual
ShuffleNet $2\times$ ($g = 3$) (Zhang et al., 2017)	26.3	–	$\sim$5	524	–	manual
NASNet-A (Zoph et al., 2018)	26.0	8.4	5.3	564	2000	RL
NASNet-B (Zoph et al., 2018)	27.2	8.7	5.3	488	2000	RL
NASNet-C (Zoph et al., 2018)	27.5	9.0	4.9	558	2000	RL
AmoebaNet-A (Real et al., 2018)	25.5	8.0	5.1	555	3150	evolution
AmoebaNet-B (Real et al., 2018)	26.0	8.5	5.3	555	3150	evolution
AmoebaNet-C (Real et al., 2018)	24.3	7.6	6.4	570	3150	evolution
PNAS (Liu et al., 2018a)	25.8	8.1	5.1	588	$\sim$225	SMBO
DARTS (searched on CIFAR-10)	26.7	8.7	4.7	574	4	gradient-based

ENAS missing!

Architecture	Perplexity valid	Perplexity test	Params (M)	Search Cost (GPU days)	Search Method
LSTM + augmented loss (Inan et al., 2017)	91.5	87.0	28	–	manual
LSTM + continuous cache pointer (Grave et al., 2016)	–	68.9	–	–	manual
LSTM (Merity et al., 2018)	69.1	66.0	33	–	manual
LSTM + skip connections (Melis et al., 2018)	69.1	65.9	24	–	manual
LSTM + 15 softmax experts (Yang et al., 2018)	66.0	63.3	33	–	manual
ENAS (Pham et al., 2018b)† (searched on PTB)	72.4	70.4	33	0.5	RL
DARTS (searched on PTB)	71.2	69.6	33	1	gradient-based

Summary

Main results

1. Proves gradient-based approach is possible and appropriate
2. Competitive results on accuracy
3. Outperforms all existing gradient-free methods in speed ?
4. Demonstrated transferability from small to large datasets:
    a. CNN: CIFAR-10 to ImageNet
    b. RNN: PTB to WikiText-2

Advantages of DARTS

1. Fast and accurate
2. No controllers
3. General enough for CNN and RNN

Discussion points:

1. Why was ENAS not compared?
2. ENAS performance comes close despite being RL
3. Why Normal and Reduction cells?

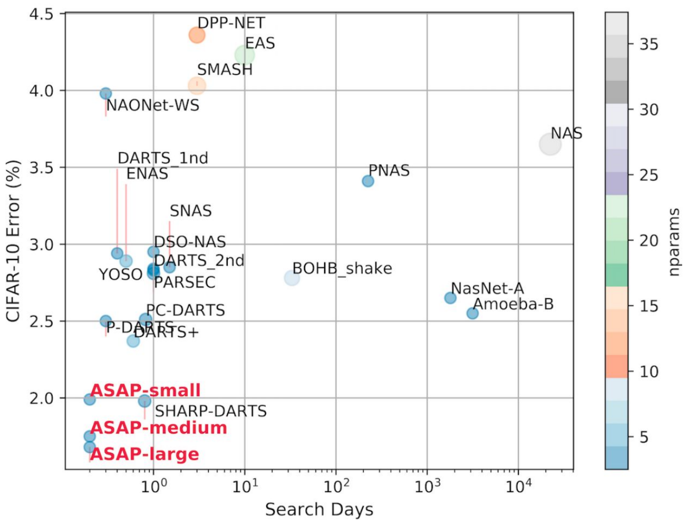
ASAP: Architecture Search, Anneal and Prune

Asaf Noy, Niv Nayman, Tal Ridnik, Nadav Zamir, Sivan Doveh, Itamar Friedman, Raja Giryes, Lihi Zelnik-Manor

AISTATS 2020

Problem Statement and Claims

- Adopts the same approach of DARTS (gradient-based)
- Argues that DARTS is not fast enough, the *post-training* pruning strategy is inefficient (*relaxation bias* [Xie et al., 2019])
- Gradual *during-training* pruning results in more efficient search
- In addition to continuity and differentiability of search space, ASAP advocates annealability for more efficient optimization.
- Claims to bring 1-4 GPU days of DART down to hours.



Method

A generalization of DARTS to annealable search space: DARTS + anneal and prune strategy

$$o \in \mathcal{O} \qquad x^{(j)} = \sum_{i<j} o^{(i,j)}(x^{(i)}) \qquad \bar{o}^{(i,j)}(\boldsymbol{x};T) \;=\; \sum_{o \in \mathcal{O}} \Phi_o(\boldsymbol{\alpha}^{(i,j)};T) \cdot o(\boldsymbol{x})$$

$$\Phi_o(\boldsymbol{\alpha}^{(i,j)};T) = \frac{\exp\left\{\frac{\boldsymbol{\alpha}_o^{(i,j)}}{T}\right\}}{\sum_{o' \in \mathcal{O}} \exp\left\{\frac{\boldsymbol{\alpha}_{o'}^{(i,j)}}{T}\right\}} \qquad \dim \alpha^{(i,j)} = |\mathcal{O}|$$

Φ_o forms a uniform (distribution) for $T \to \infty$ and sparse for $T \to 0$

Annealing schedule: $T(t) = T_0 \beta^t$

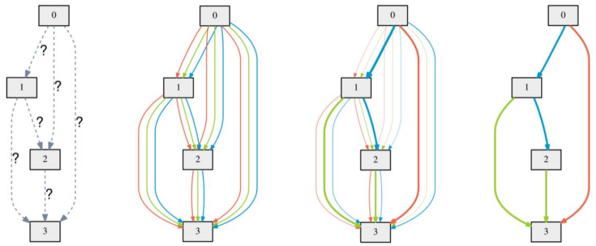
Threshold policy: $\Theta \equiv \theta_0$

Stopping condition: when only a single operation is left in $\mathcal{O}$ for a (i,j)

Key to success is the balance between $T(t)$ and Θ

Algorithm 1 ASAP for a single Mixed Operation

Input: Operations $o_i \in \mathcal{O}\ \ i \in \{1,..,N\}$,
Annealing schedule T_t,
Grace-temperature τ,
Threshold policy θ_t,
Init: $\boldsymbol{\alpha}_i \leftarrow 0,\ \ i \in \{1,..,N\}$.
while $|\mathcal{O}| > 1$ **do**
  Update $\boldsymbol{\omega}$ by descent step over $\nabla_{\boldsymbol{\omega}} \mathcal{L}_{\text{train}}(\boldsymbol{\omega}, \boldsymbol{\alpha}; T_t)$
  if $T_t < \tau$ **then**
    Update $\boldsymbol{\alpha}$ by descent step over $\nabla_{\boldsymbol{\alpha}} \mathcal{L}_{\text{val}}(\boldsymbol{\omega}, \boldsymbol{\alpha}; T_t)$
    for each $o_i \in \mathcal{O}$ such that $\Phi_{o_i}(\boldsymbol{\alpha}; T_t) < \theta_t$ **do**
      $\mathcal{O} = \mathcal{O} \setminus \{o_i\}$
    end for
  end if
  Update T_t
  Update θ_t
end while
return $\mathcal{O}$

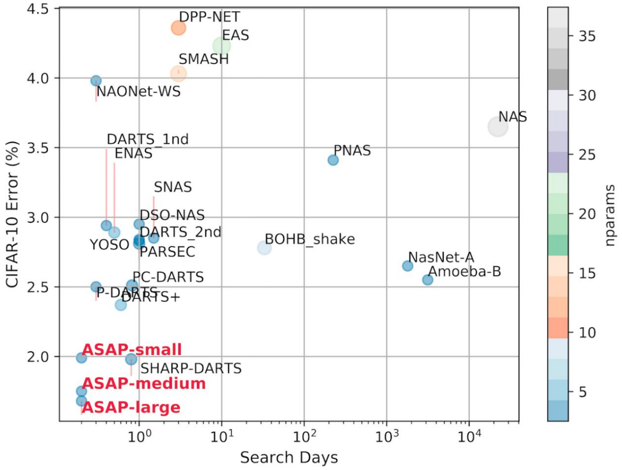


Experiments

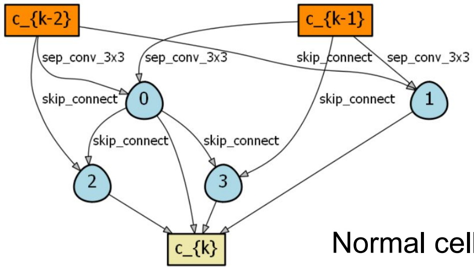
Follows the same experiment design of DARTS:

Fix outer structure ⇒ search operations in a cell ⇒ scale up outer structure ⇒ train CNN

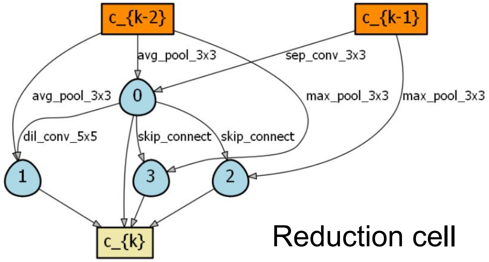
Architecture search in a small structure on CIFAR-10 took only 4.8 hours on single GPU.



Results on CIFAR-10 (no transfer)



Normal cell



Reduction cell

Learned cells on CIFAR-10

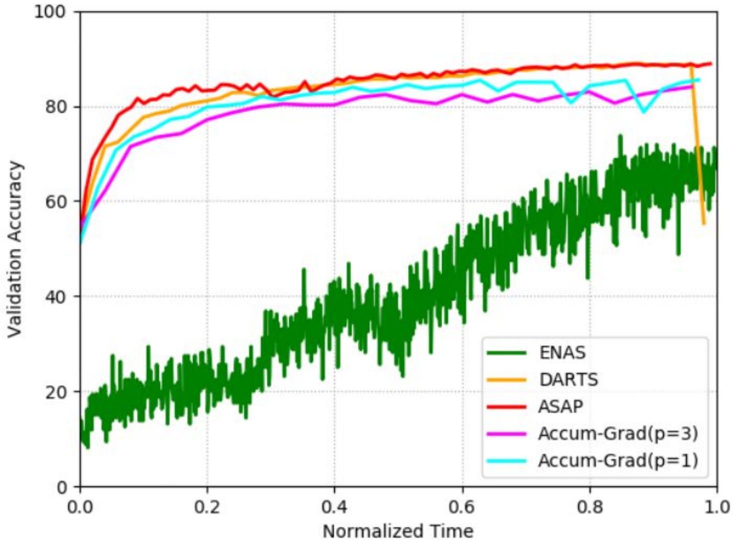
Experiments

Transferability tests:

Architecture	CINIC-10 Error(%)	FREIBURG Error(%)	CIFAR-100 Error(%)	SVHN Error(%)	FMNIST Error(%)	ImageNet Error(%)	Search cost ↓
Known SotA	8.6	21.1	8.7	1.02	3.65	15.7	-
AmoebaNet-A	7.18	11.8	15.9	1.93	3.8	**24.3**	3150
NASNet	6.93	13.4	15.8	1.96	3.71	26.0	1800
PNAS	7.03	12.3	15.9	1.83	3.72	25.8	150
SNAS	7.13	14.7	16.5	1.98	3.73	27.3	1.5
DARTS-Rev1	7.05	11.4	15.8	1.94	3.74	26.9	1
DARTS-Rev2	6.88	10.8	15.7	1.85	**3.68**	26.7	1
ASAP	**6.83**	**10.7**	**15.6**	**1.81**	3.73	24.4	**0.2**

Experiments

Effect of *relaxation-bias*:

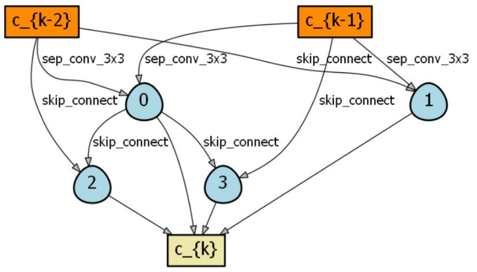


Summary

- A generalization of DARTS into annealable search space
- ASAP anneals and prunes the connection weights within the cell in a continuous manner
- Based on the insight that pruning during training reduces complexity and speeds up search.
- Theoretical results are available that enable good tradeoff between annealing schedule and threshold policy
- Achieves better training speed than DARTS while maintaining good accuracy

Discussion points:

1. The pruning strategy does not account for too many parents for a node in the cell. DARTS fixed this manually (k=2).
2. In spite of not fixing the above, all nodes in the learned cells have exactly two parents. This is a mystery!



References

[Elshawi et al., 2019] Elshawi, Radwa, Mohamed Maher, and Sherif Sakr. "Automated machine learning: State-of-the-art and open challenges." *arXiv preprint arXiv:1906.02287* (2019).
[Zoph et al., 2018] Zoph, Barret, et al. "Learning transferable architectures for scalable image recognition." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2018.
[Real et al., 2018] Real, Esteban, et al. "Regularized evolution for image classifier architecture search." *Proceedings of the aaai conference on artificial intelligence*. Vol. 33. 2019.
[Xie et al., 2019] Sirui Xie, Hehui Zheng, Chunxiao Liu, and Liang Lin. Snas: Stochastic neural architecture search. In *International Conference on Learning Representations* (ICLR), 2019.