Deep Learning Optimisé - Jean Zay

Optimisation des hyperparamètres

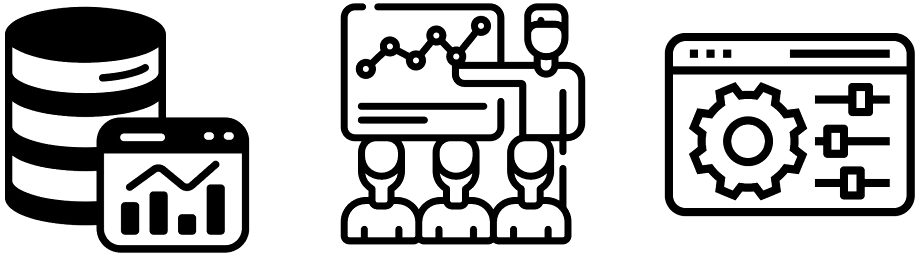
cnrs
Institut du Développement et des Ressources en Informatique Scientifique

HPO = Hyperparameter Optimisation

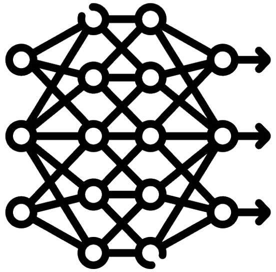
Hyperparameters

In machine learning, a hyperparameter is **a parameter whose value is used to control the learning process**. By contrast, the values of other parameters (typically node weights) are derived via training.

Hyperparameters

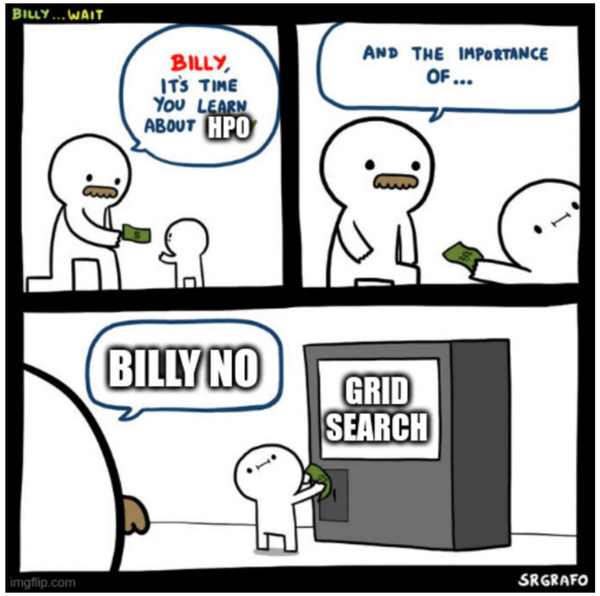


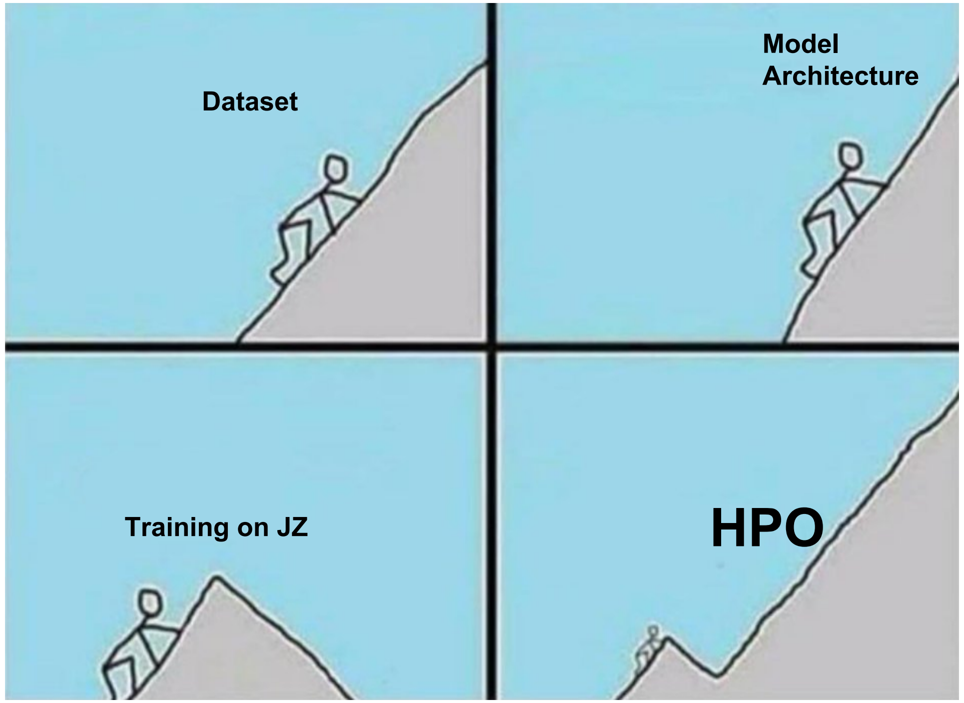
Parameters



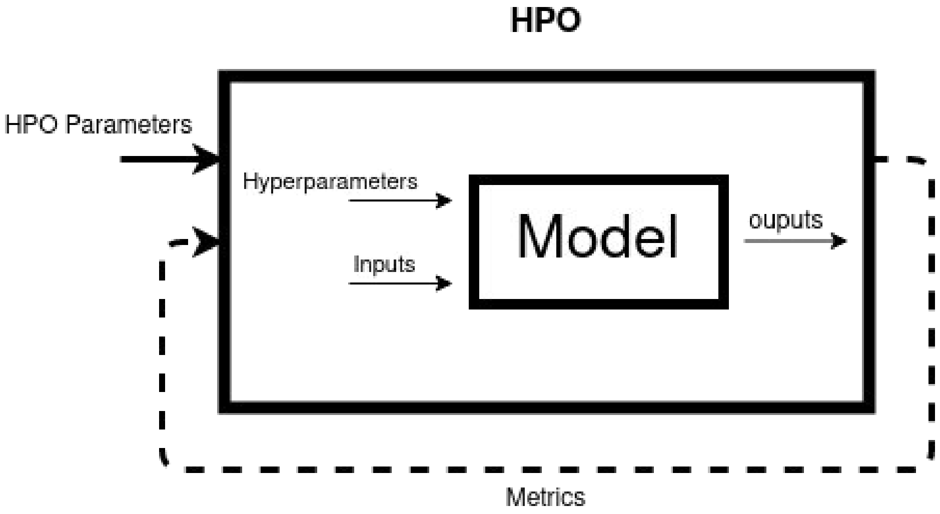
HPO : Hyperparameter Optimisation

Machine learning algorithms are highly configurable by their hyperparameters.
These parameters often substantially influence the complexity, behavior, speed as well as other aspects of the learner, and their values must be selected with care in order to achieve optimal performance.
Human trial-and-error to select these values is time-consuming, often somewhat biased, error-prone and computationally irreproducible.





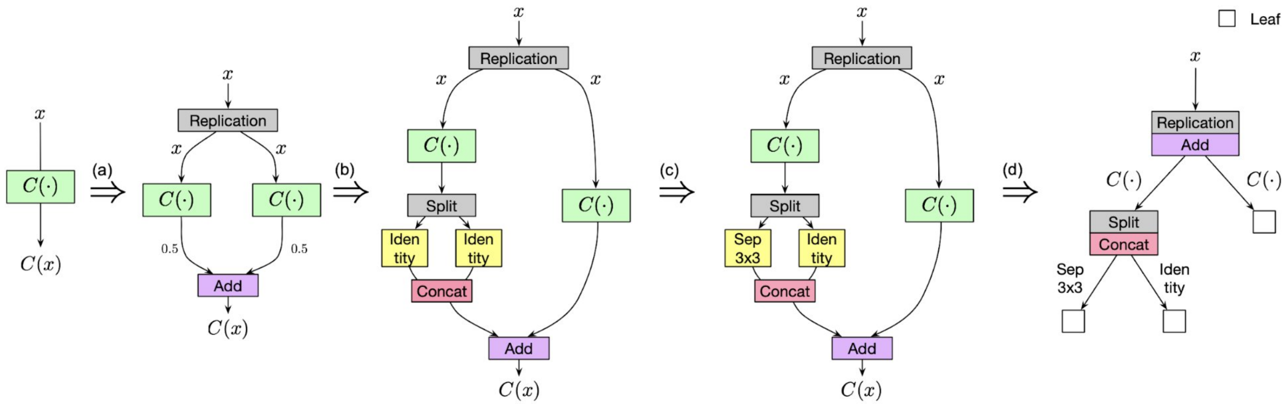
HPO



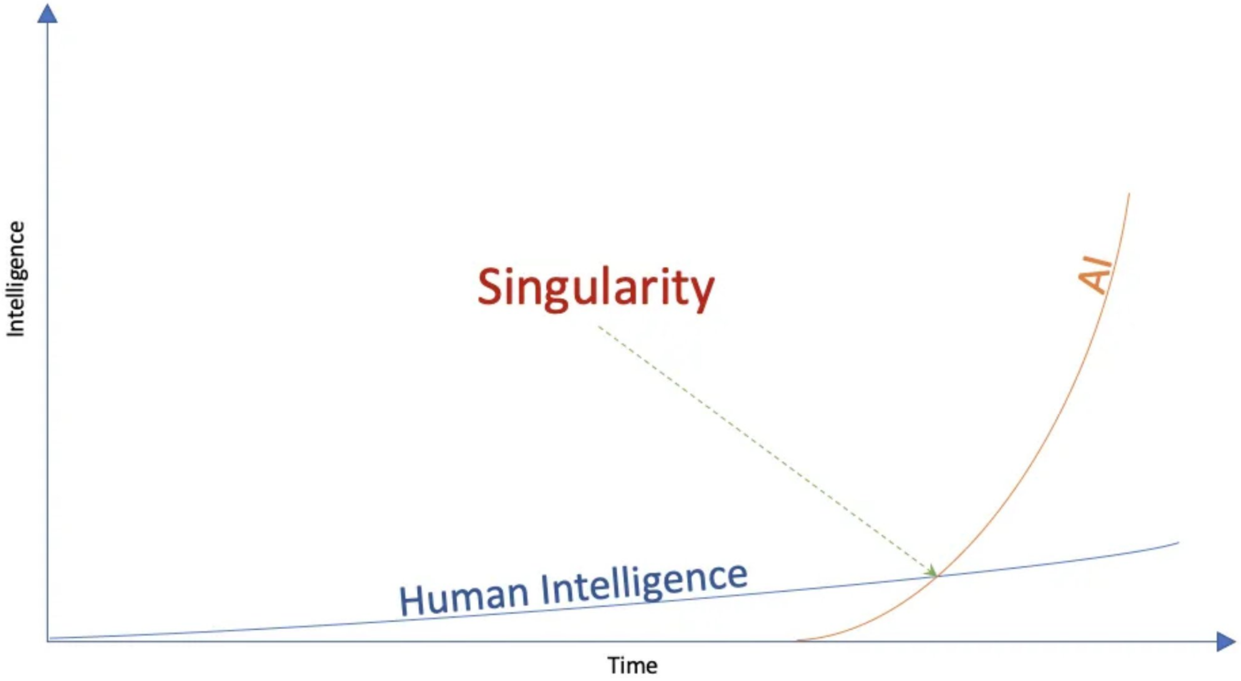
Hyperparameter Optimization == Bi-Level optimization problem

Related Problems

- Neural Architecture Search **(NAS)**
- Algorithm Selection and traditional Meta-Learning
- Algorithm configuration **(AC)**
- Dynamic Algorithm Configuration **(DAC)**
- Learning to learn and to optimize



A Comprehensive Survey of Neural Architecture Search: Challenges and Solution (https://arxiv.org/pdf/2006.02903.pdf)



Fastest wheel change on a moving car - Guinness World Records

Search Algorithms / Samplers

Basic ◂

Manual, Grid Search, Random Search

Bayesian Optimisation ◂

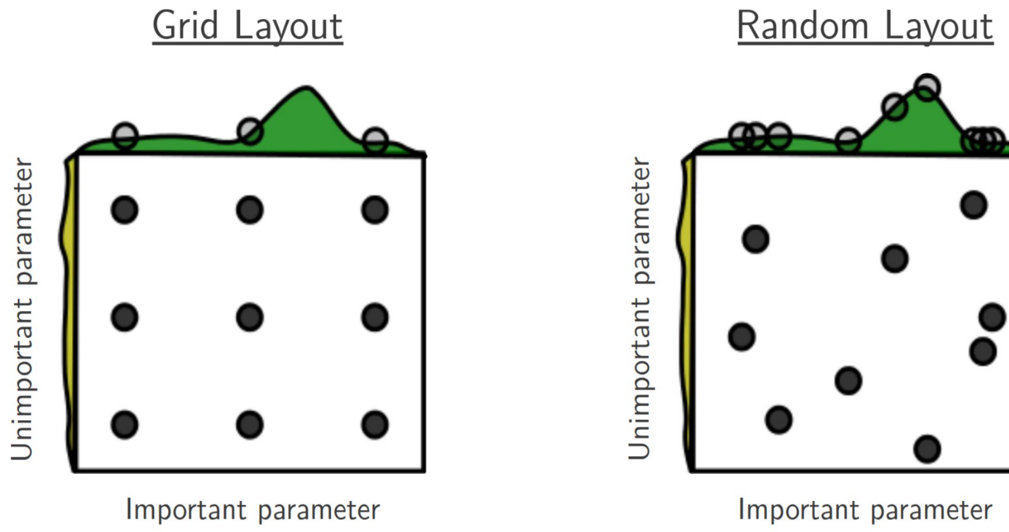
Tree-structured Parzen Estimator, Gaussian Process

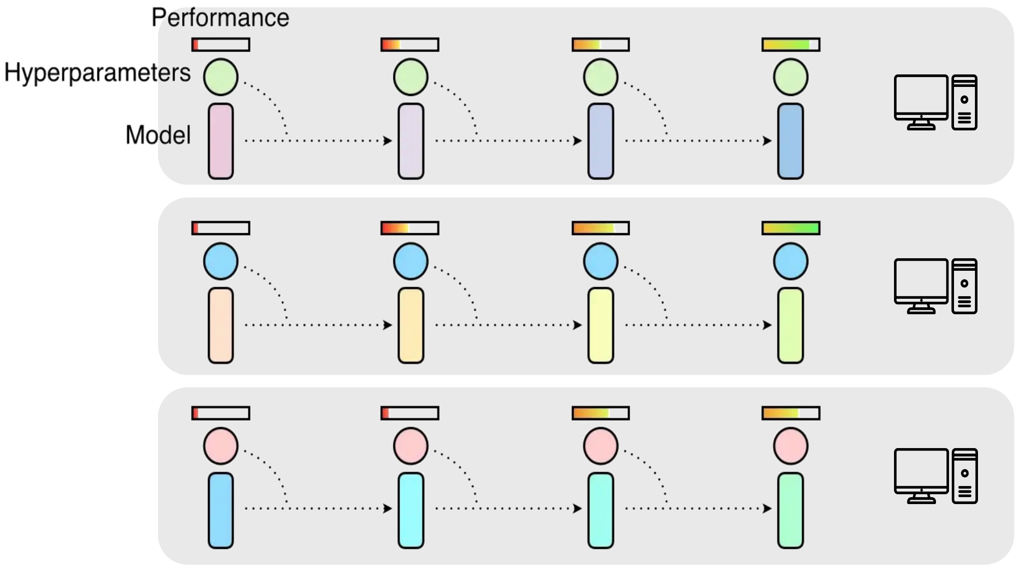
Heuristic ◂

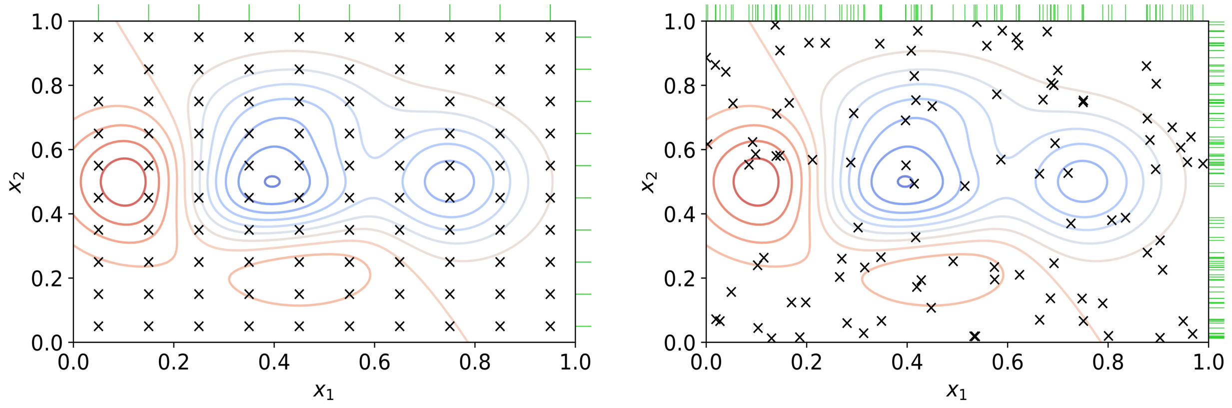
Genetic Algorithm, Particle Swarm Optimization

Gradient-based Optimization ◂

Basic : Grid & Random Search

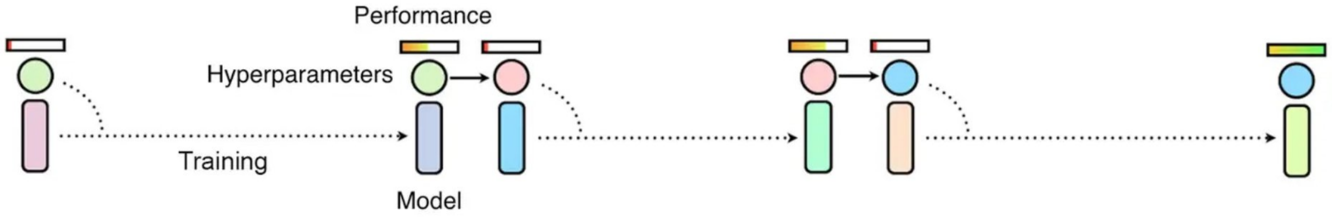


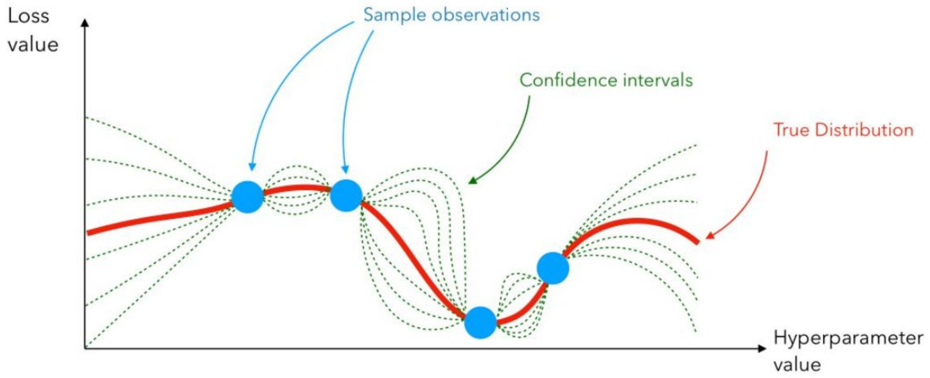




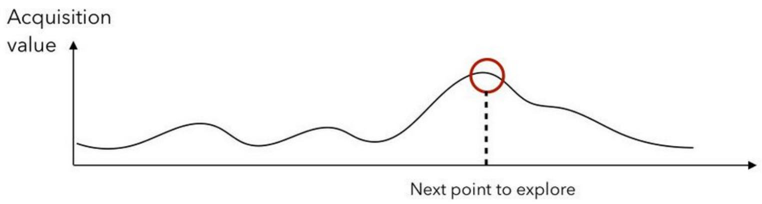
- Independent tests (which can be parallelized) which test a combination of hyperparameters.
- Very costly in resources and no guarantee of improved results.
- Random search is better for high dimensional space

Bayesian Optimization : TPE & GP



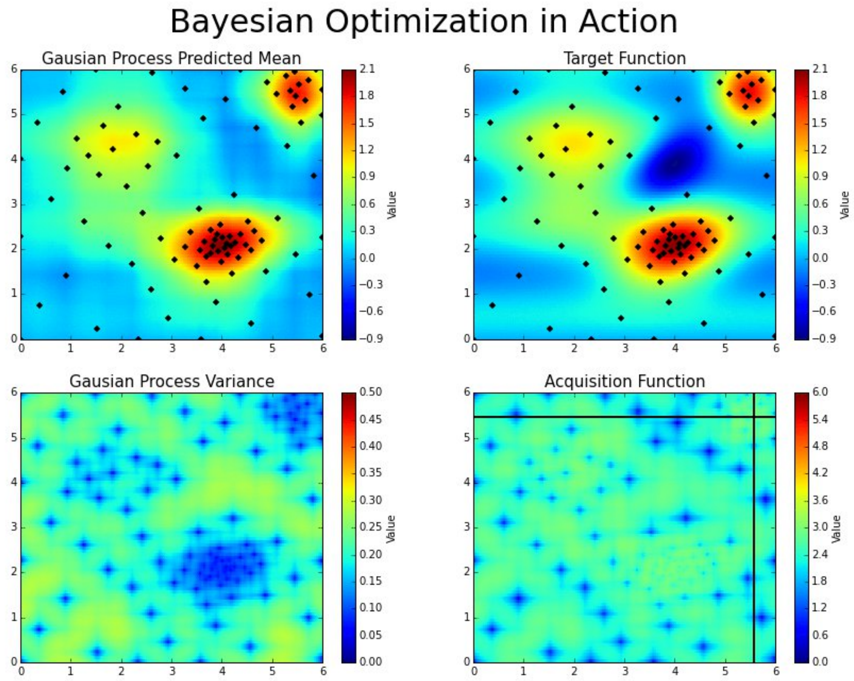


Expected metric score according to Hyper-parameters

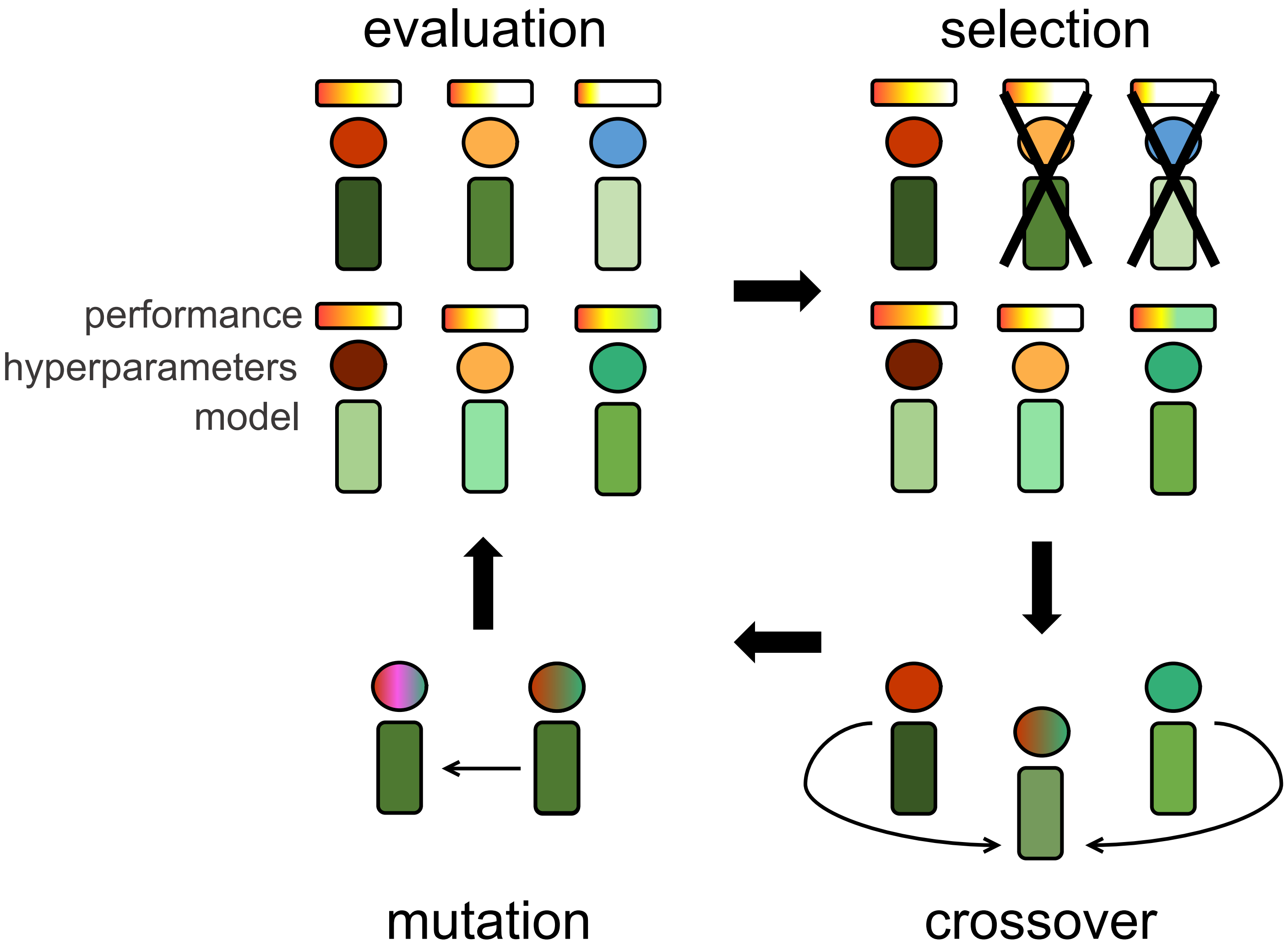


Maximize Acquisition function e.g. Expected Improvement

- Tree Parzen Estimator / Gaussian Process
- Sequential but allows to quickly find the global optimum.
- Proposes a new set of hyper parameters based on the scores obtained by the previous ones tested.



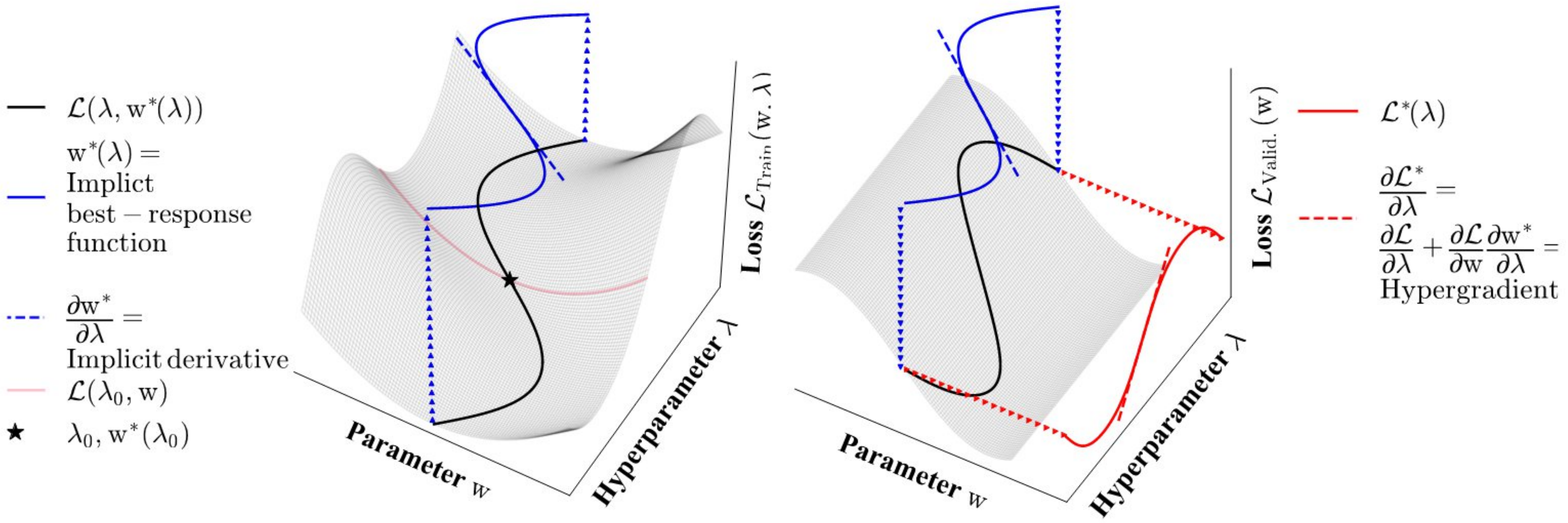
Heuristic : Evolutionary Optimization



- Bio-inspired
- Can have fatal mutation

- **Genetic Algorithm (GA)**
- **Genetic Programming (GP)**
- **Evolution Strategy (ES)**
- **Particle Swarm Optimization (PSO)**
- **Estimation of Distribution Algorithms (EDA)**

Gradient-based optimization



Optimizing Millions of Hyperparameters by Implicit Differentiation
(https://arxiv.org/pdf/1911.02590.pdf)

- High dimensionality
- Bi-level optimisation

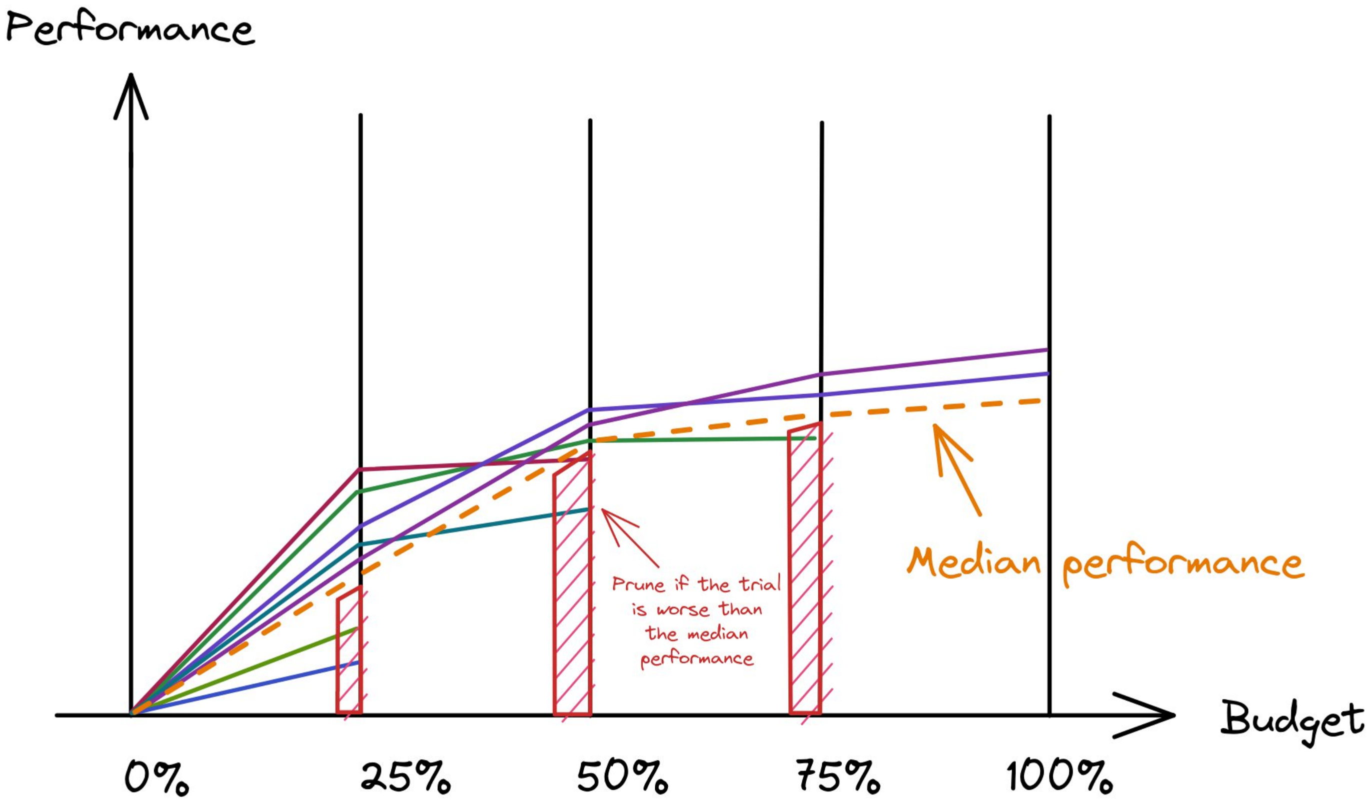
Schedulers Algorithms / Pruners

Early Stopping ◂

SHA/ASHA ◂

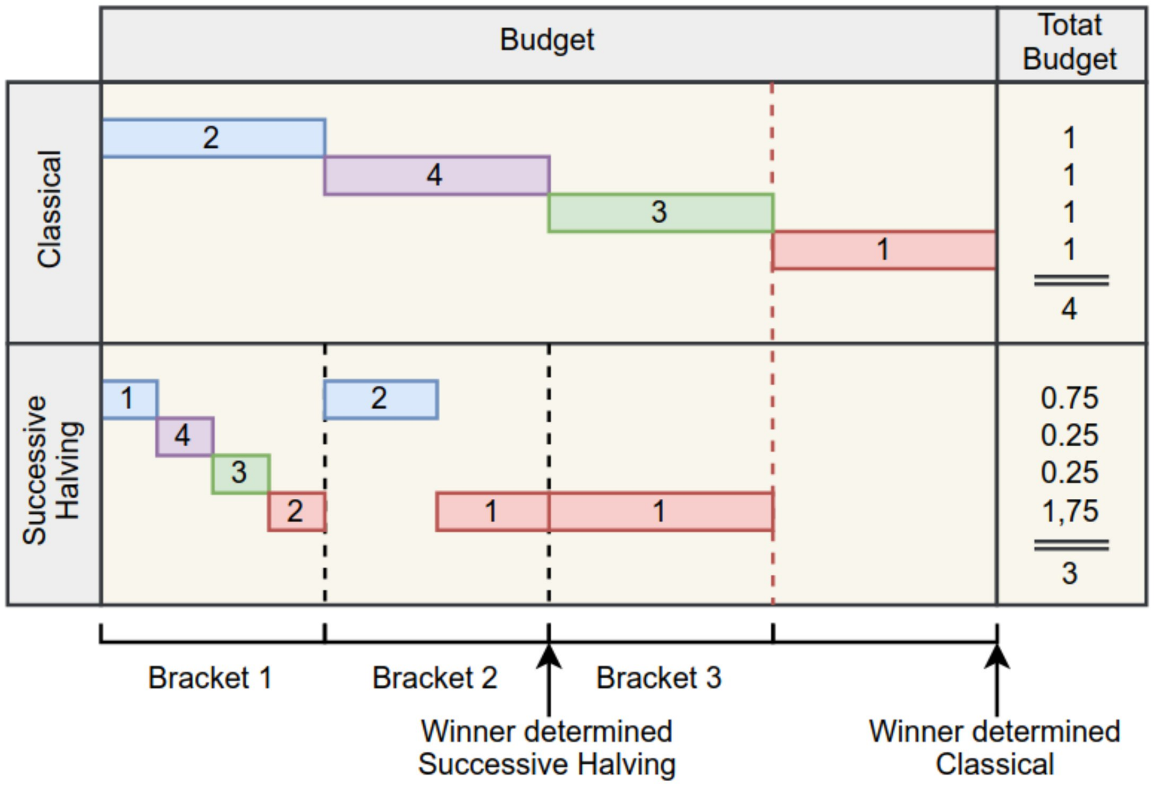
HyperBand ◂

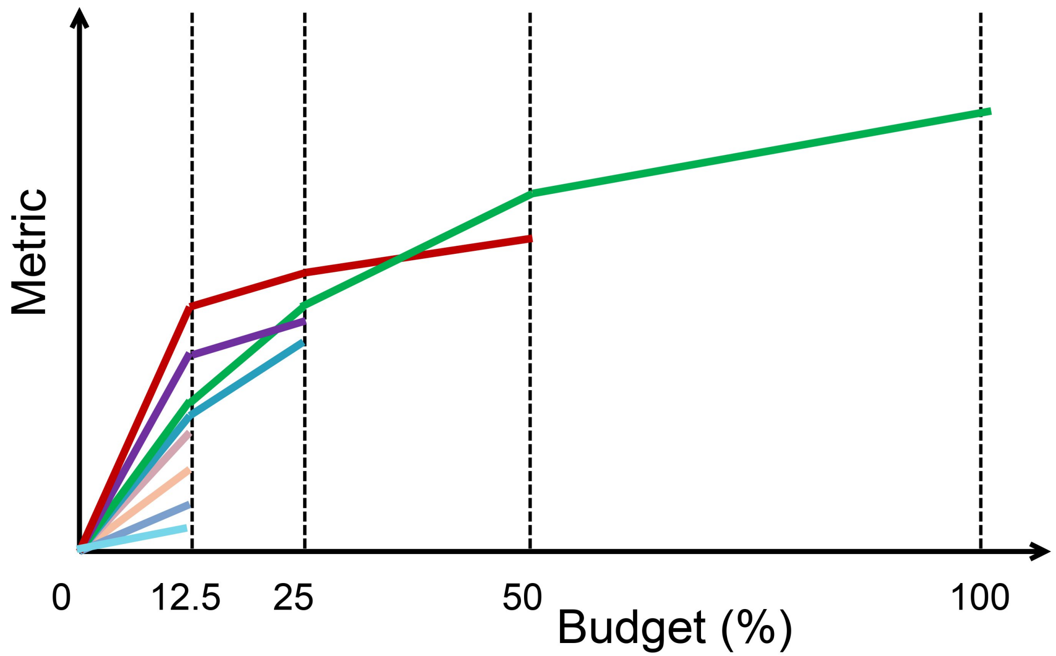
Early Stopping



- Easy to implement
- Save ressources & make automatic selection
- Can be with acc%, time%, rank%, etc

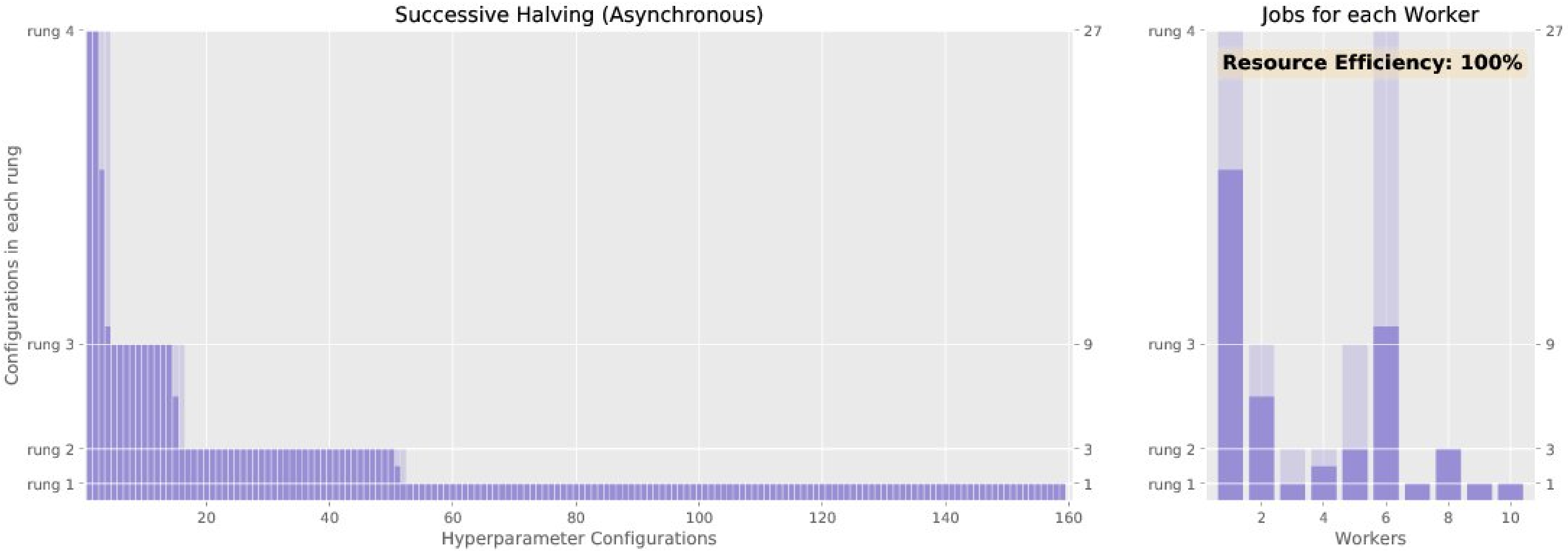
SHA : Successive Halving Algorithm





- For sequentials trials
- Works well with small or medium model -> Trials must be fast !

ASHA



Successive Halving (Asynchronous)
Configurations in each rung
rung 4
rung 3
rung 2
rung 1
27
9
3
1
20
40
60
80
100
120
140
160
Hyperparameter Configurations
Jobs for each Worker
Resource Efficiency: 100%
2
4
6
8
10
Workers

Hyperband

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**
  $n = \lceil \frac{B}{R} \frac{\eta^s}{(s+1)} \rceil, \quad r = R\eta^{-s}$
  // 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.*

i	$s=4$ n_i	$s=4$ r_i	$s=3$ n_i	$s=3$ r_i	$s=2$ n_i	$s=2$ r_i	$s=1$ n_i	$s=1$ r_i	$s=0$ n_i	$s=0$ r_i
0	81	1	27	3	9	9	6	27	5	81
1	27	3	9	9	3	27	2	81		
2	9	9	3	27	1	81				
3	3	27	1	81						
4	1	81								

Table 1: Values of n_i and r_i for the brackets of HYPERBAND when $R = 81$ and $\eta = 3$.

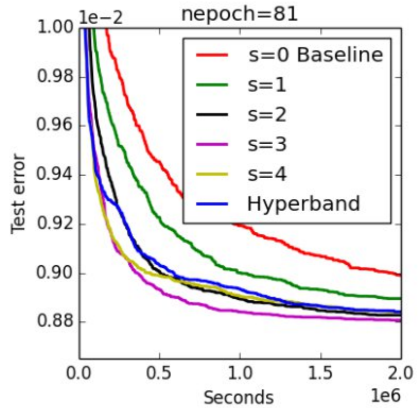
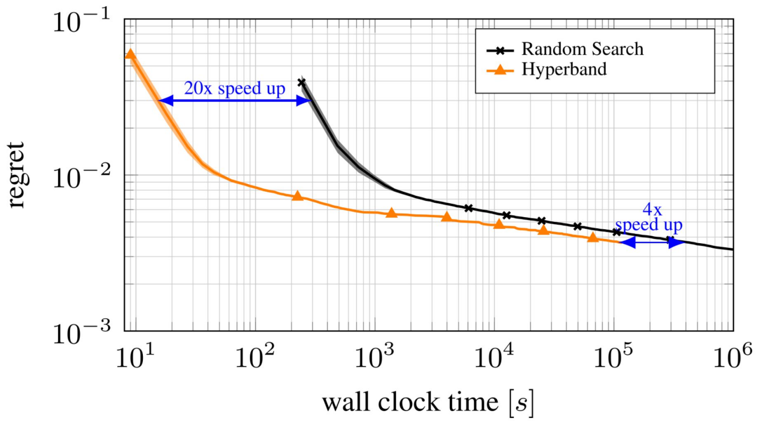


Figure 2: Performance of individual brackets s and HYPERBAND.



- Repeatedly calls SuccessiveHalving but mitigate it's drawbacks
- Limited convergence

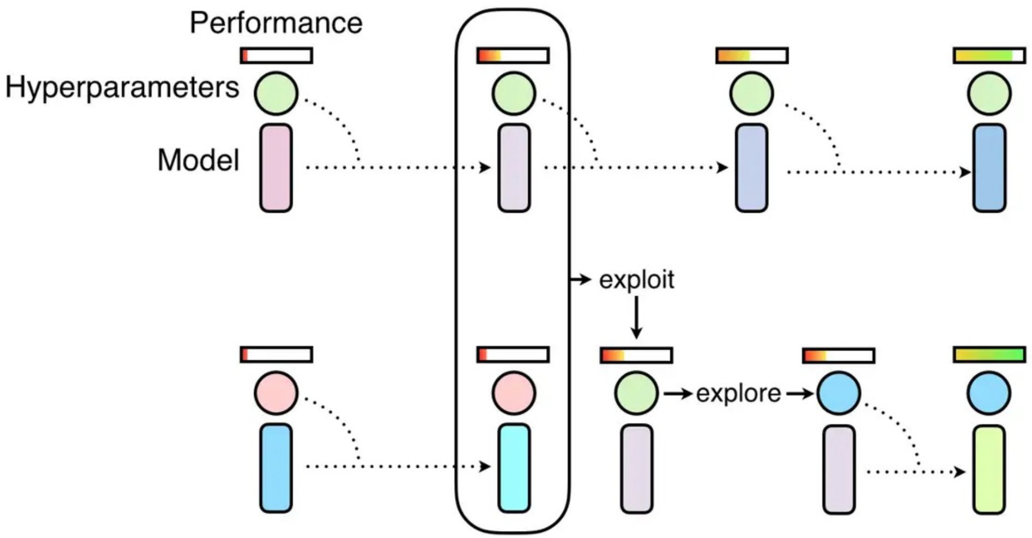
Advanced Algorithms

Hybrid time !

PBT ◂

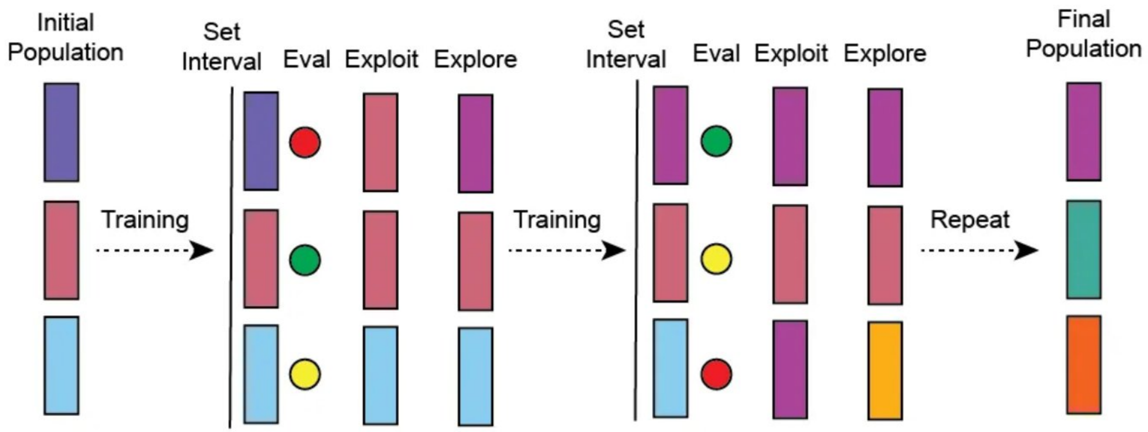
BOHB, DEHB ◂

PBT : Population Based Training



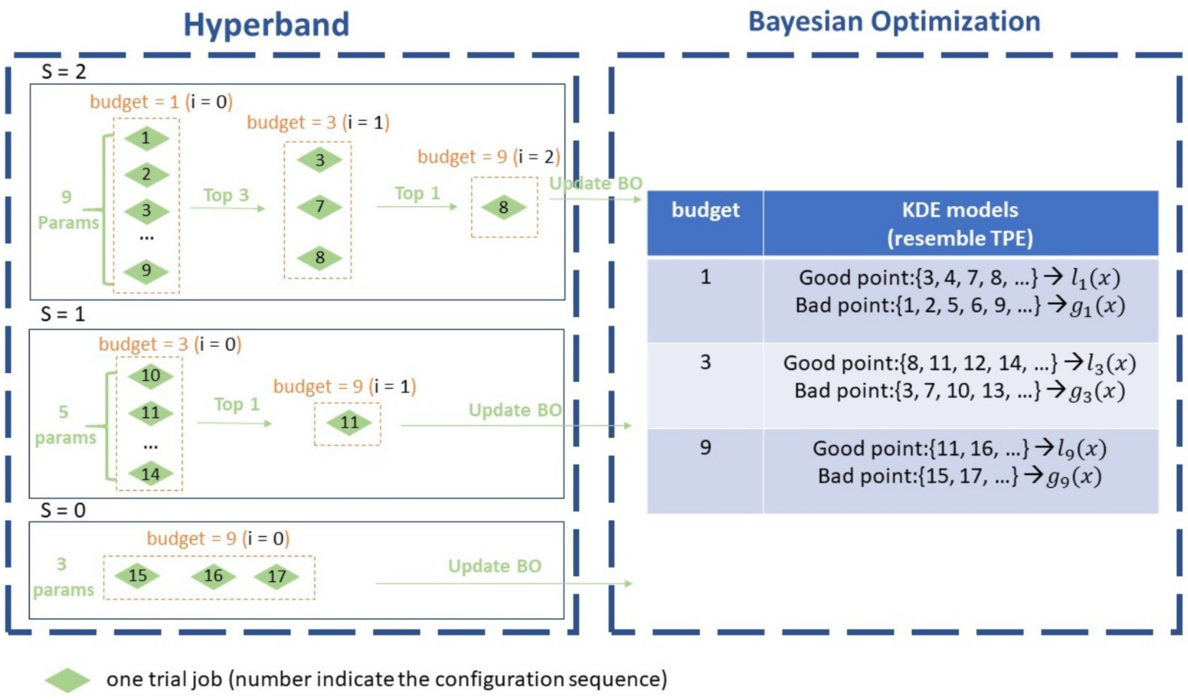
- Research and optimization of hyper parameters during training
- For large models with long and poorly parallelizable tests on a few machines.

- **Exploit** = Copy of the weights of the best model
- **Explore** = Bayesian Optimization

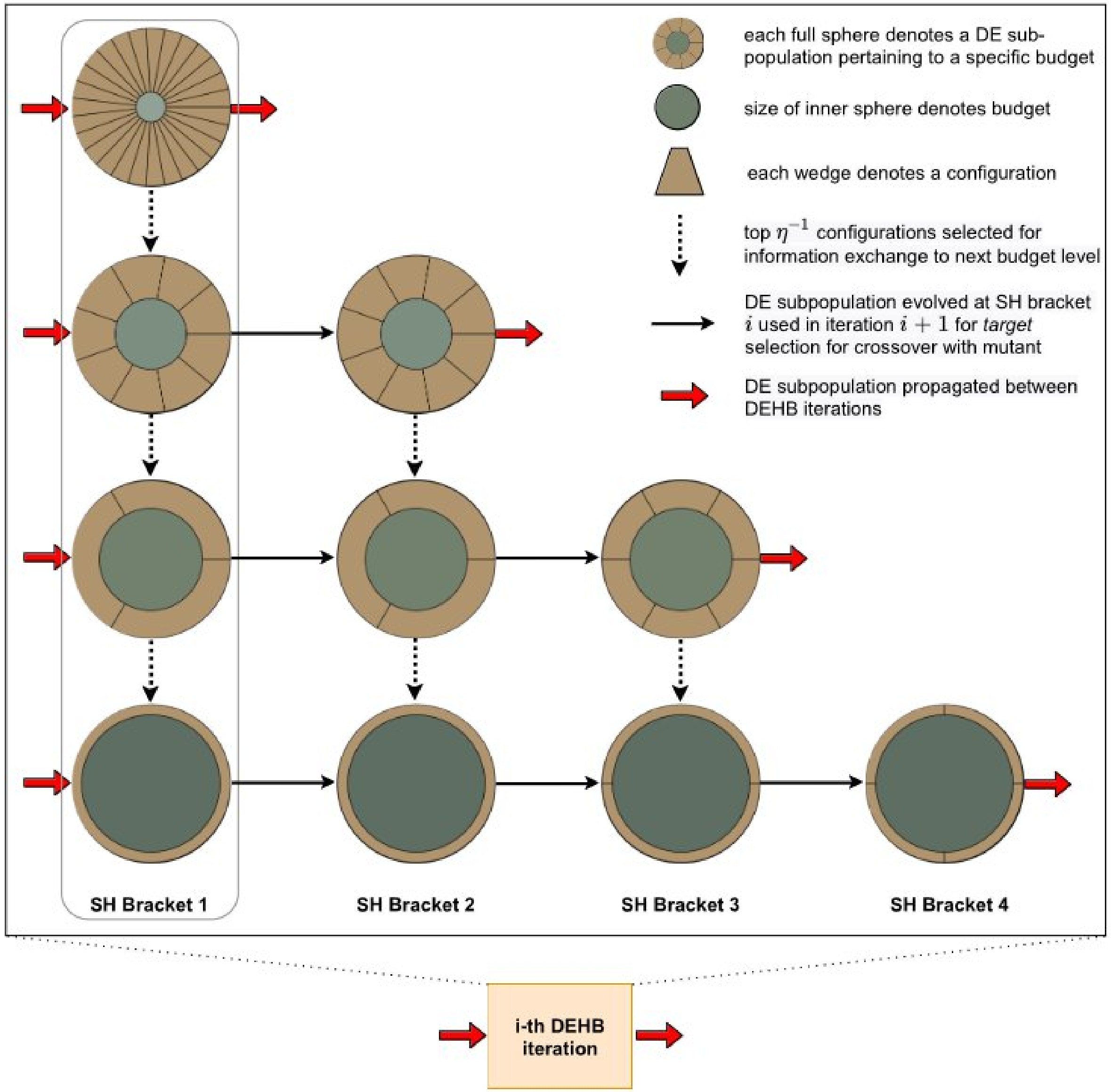


BOHB, DEHB

BOHB : Bayesian Optimization Hyperband

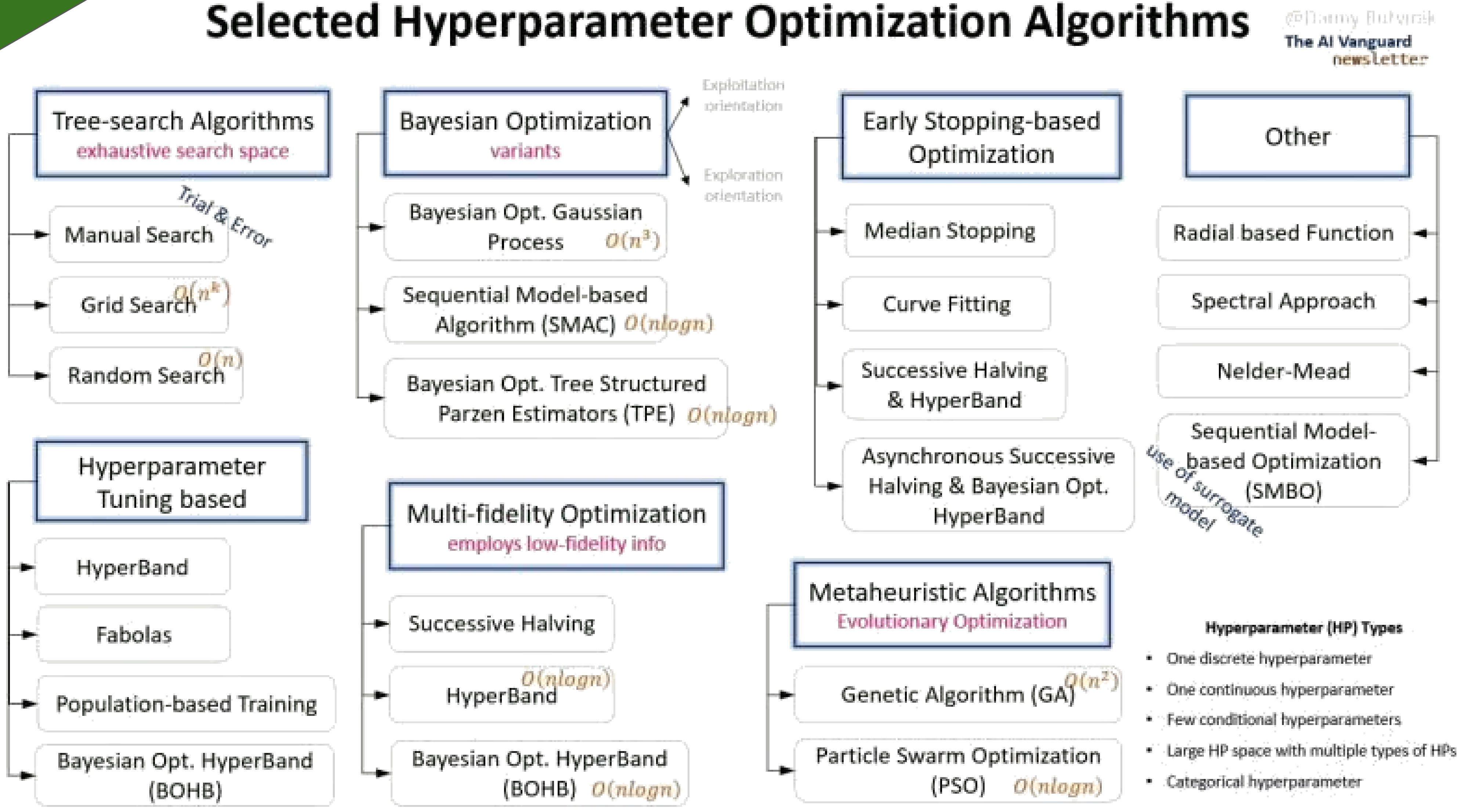


DEHB : Differential Evolution Hyperband



Summary

Selected Hyperparameter Optimization Algorithms



Have the right tools

HPO frameworks ◂

Visualisation & Experiments Tracking ◂

HPO Frameworks & tools

Hydra

- Based on config file
- Easy to use
- Not only used for ML/DL

OPTUNA

- Work with an objective function
- Efficient Optimization Algorithms

RAY tune

- Scalable HPO framework
- State of the art algorithms (PBT)
- Integrates with a wide range of additional HPO tools

Experiments tracking

mlflow ou Weights & Biases +

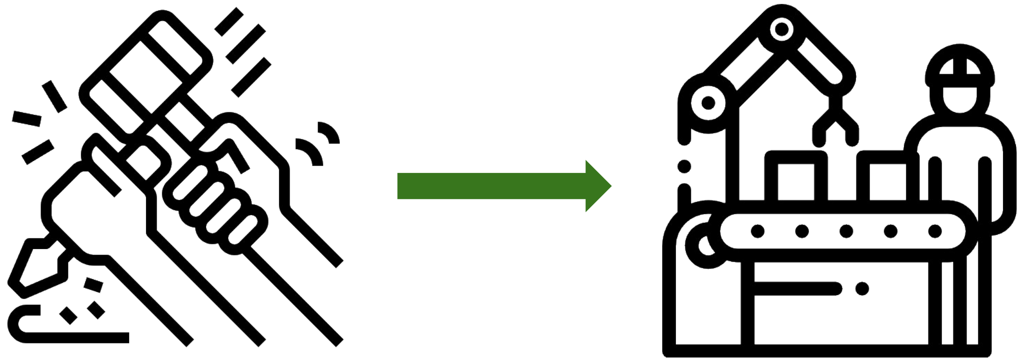
Source Control git

Data Version Control DVC

Advantages :

- allows you to save and order the results
- allows easy comparison and visualization of results
- provides all the information needed to reproduce the results

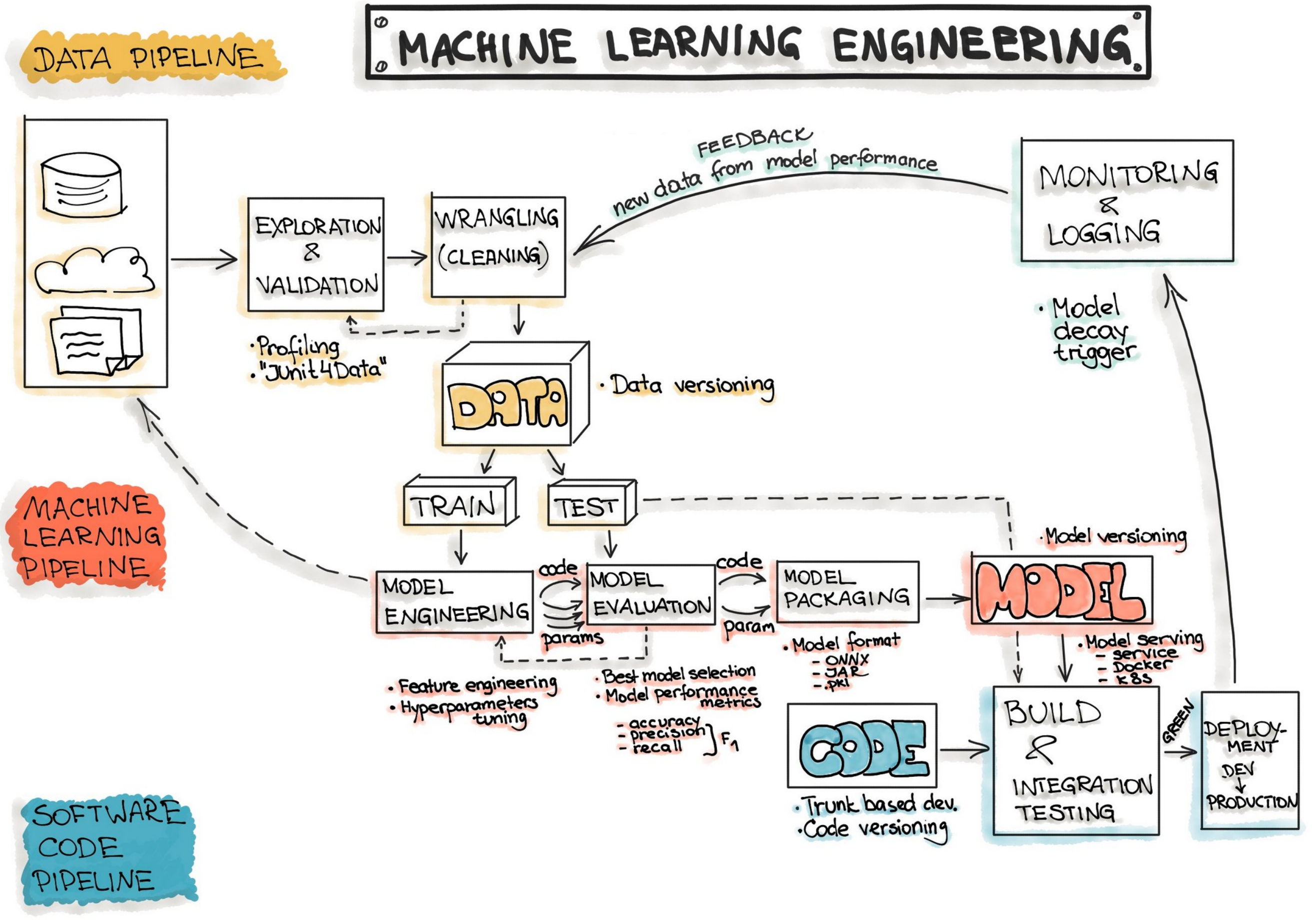
HPO and MLOps



- As soon as our HPO requires a lot of resources (time, money or both) it is necessary to scale up and industrialize the experience process.
- Taking inspiration from MLOps processes and tools is a good start

Kubeflow

mlflow™



https://ml-ops.org/content/end-to-end-ml-workflow

Sources

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- Population Based Training : https://www.deepmind.com/blog/population-based-training-of-neural-networks