Hyperparameter Optimization

Intro

- Every machine learning has *hyperparameters*.
- Tuning hyperparameters is, at the very least, annoying.
- True end-to-end learning should not require a costly expert playing around with hyperparameters!

Definition: Hyperparameter optimization (HPO)

- $D = (D_{train}, D_{valid})$ our data
- A an algorithm
- Λ the set of possible hyperparameters (configuration space)
- $\mathcal{L}(A_\lambda, D_{train}, D_{valid})$ loss function of A, with $\lambda \in \Lambda$.
- **Goal:** find λ^* such that:

$$\lambda^* \in \operatorname{argmin}_{\lambda \in \Lambda} \mathcal{L}(A_\lambda, D_{train}, D_{valid}).$$

Devil in the details

- The reality is that we often have a **complex configuration space** with a mixture of continuous, integer, categorical and conditional components.

Configuration space (cont.)

- Continuous
  - Learning rates (e.g. in deep learning).
- Integer
  - Number of trees in GBM/random forests.
- Categorical
  - Activation functions (ReLU, LeakyReLU, $\tanh$).
  - Operator ($\text{conv}3 \times 3$, max pool layer).
- Conditional
  - Hyperparams that are only available if something else was chosen (e.g. number of trees if classifier = RF).

Def: Combined Algorithm Selection and Hyperparameter Optimization (CASH)

- $D = (D_{train}, D_{valid})$ our data
- $\mathcal{A} = \{A_1, A_2, \ldots A_n\}$ a set of algorithms.
- Λ_i the configuration space for A_i.
- $\mathcal{L}(A_{i,\lambda}, D_{train}, D_{valid})$ loss function of A_i, with $\lambda \in \Lambda_i$.
- **Goal:** find A_*, λ^* such that:

$$A_{*,\lambda^*} \in \mathrm{argmin}_{i,\lambda \in \{1,2,\ldots n\} \times \Lambda} \mathcal{L}(A_{i,\lambda}, D_{train}, D_{valid}).$$

Approaches

- Black-box Optimization.
- Bayesian Optimization.
- Sequential Model-based Algorithm Configuration (SMAC).
- Tree-structured Parzen Estimator (TPE).

Black-box Optimization

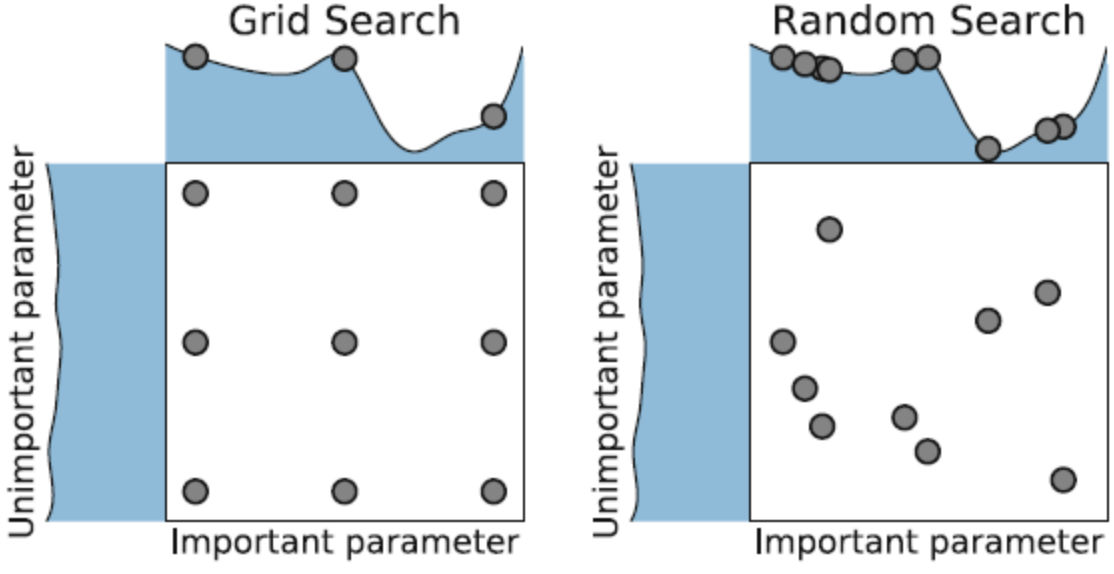
- Ignore everything, focus on minimizing $\mathcal{L}(\lambda)$.
- Two alternatives: grid search, (pure) random search.

Grid search

- The user provides a range of values for each hyperparameter.
- The function is evaluated in the Cartesian product of these lists.
- Number of function evaluations grows exponentially with the dimension of the hyperparameter space: if you have n hyperparameters and choose two values, you already need 2^n evaluations!.

Random search

- The user provides a range of values for each hyperparameter.
- The function is evaluated in a sample over the cartesian product.
- Easier parallelization.
- Useful baseline, since it does not make any assumptions on the underlying machine learning algorithm being used.
- Can do better than grid search:



Population-based methods

- Not random search (?).
- Genetic algorithms, evolutionary algorithms, evolutionary strategies, particle swarm optimization.
- CMA-ES (covariance matrix adaption evolutionary strategy).
- Natural Evolution Strategies.

Cross-Entropy Method (CEM)

```
for it in range(n_iter):
    # Sample parameter vectors
    las = np.random.normal(la_mean, la_std, (bsize,dim_la))
    rewards = [f(la) for la in las]
    # Get elite parameters
    n_elite = int(batch_size * elite_frac)
    elite_ids = np.argsort(rewards)[bsize-n_elite:bsize]
    elite_las = [las[i] for i in elite_ids]
    # Update la_mean, la_std
    la_mean = np.mean(elite_las,axis=0)
    la_std = np.std(elite_las,axis=0)
    print(solution, la_mean)
```

Beyond random search

Bayesian Optimization

- Two key ingredients:
  - a probabilistic surrogate model.
  - an acquisition function to decide which point to evaluate next.
- A popular candidate for acquisition function is the *expected improvement*.

Bayesian Optimization (cont.)

- In each iteration, the surrogate model is fitted to all observations of the target function made so far.
- Then the acquisition function determines the utility of different candidate points.
- Compared to evaluating the expensive blackbox function, the acquisition function is cheap to compute and can therefore be thoroughly optimized.

Example: Random search vs Gaussian Processes

Beyond Bayesian Optimization

Downsides of BO

- Scale cubically in the number of data points.
- Hard to parallelize, unlike random search or many black-box methods.
- Focus instead on hyperparameter *evaluation* rather than *selection*.

Successive halving

- **Idea:** Kill dead ends quickly.
- Try n hyperparameters for some fixed time T.
- Then keep the $n/2$ best hyperparameter settings and run for time $2T$.
- Repeating this r times, we end up with $n/2^r$ configurations.
- We get exponentially more time for testing better configurations.

Successive halving (cont.)

- **Downside:** Some configurations can be bad on the beginning, but then improve. An impatient algorithm will not find them.
- In practice, we find that:
  - Sometimes we need more time to test few configurations.
  - Some other times we need to test more configurations for less time.

Hyperband

- **Idea:** do grid search over n, the amount of hyperparameter configurations.
- All configurations get a minimum amount of resources at the beginning, before being discarded.
- As you reduce the number of configurations, the testing time increases.

Results

- Training LeNet on CIFAR-10, MNIST and SVHN.
- Hyperband is 20x faster than random search, second best competitor is 7x faster.
- **Warning:** Computation budget of 1 year of GPU hours.

References

- Successive halving implementation in sklearn.
- Comparison between Hyperband and Successive Halving
- Hyperband Implementation.
- Original Hyperband paper
- Blog post from Hyperband authors.