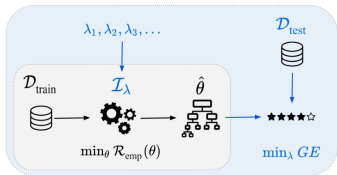


Introduction to Machine Learning

Hyperparameter Tuning

Problem Definition



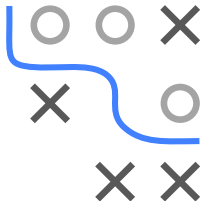
Learning goals

- Definition of HPO objective and components
- Understand its properties
- What makes tuning challenging

HYPERPARAMETER OPTIMIZATION

Hyperparameters (HP) λ are parameters that are *inputs* to learner \mathcal{I} which performs ERM on training data set to find optimal **model parameters** θ . HPs can influence the generalization performance in a non-trivial and subtle way.

Hyperparameter optimization (HPO) / Tuning is the process of finding a well-performing hyperparameter configuration (HPC) $\lambda \in \tilde{\Lambda}$ for an learner \mathcal{I}_λ .



OBJECTIVE AND SEARCH SPACE

Search space $\tilde{\Lambda} \subset \Lambda$ with all optimized HPs and ranges:

$$\tilde{\Lambda} = \tilde{\Lambda}_1 \times \tilde{\Lambda}_2 \times \cdots \times \tilde{\Lambda}_I$$

where $\tilde{\Lambda}_i$ is a bounded subset of the domain of the i-th HP Λ_i , and can be either continuous, discrete, or categorical.



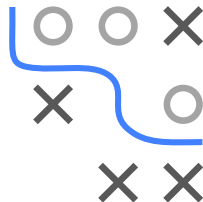
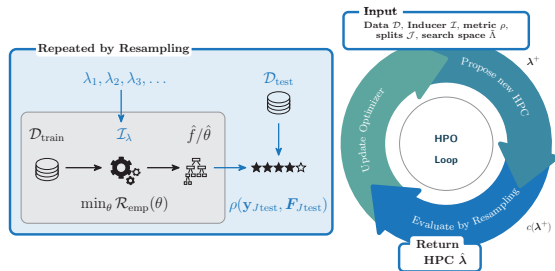
The general HPO problem is defined as:

$$\lambda^* \in \arg \min_{\lambda \in \tilde{\Lambda}} c(\lambda) = \arg \min_{\lambda \in \tilde{\Lambda}} \widehat{\text{GE}}(\mathcal{I}, \mathcal{J}, \rho, \lambda)$$

with λ^* as theoretical optimum, and $c(\lambda)$ is short for estim. gen. error when \mathcal{I} , resampling splits \mathcal{J} , performance measure ρ are fixed.

OBJECTIVE AND SEARCH SPACE

$$\lambda^* \in \arg \min_{\lambda \in \tilde{\Lambda}} c(\lambda) = \arg \min_{\lambda \in \tilde{\Lambda}} \widehat{GE}(\mathcal{I}, \mathcal{J}, \rho, \lambda)$$



- Evals are stored in **archive**

$\mathcal{A} = ((\lambda^{(1)}, c(\lambda^{(1)})), (\lambda^{(2)}, c(\lambda^{(2)})), \dots)$, with
 $\mathcal{A}^{[t+1]} = \mathcal{A}^{[t]} \cup (\lambda^+, c(\lambda^+))$.

- We can define tuner as function $\tau : (\mathcal{D}, \mathcal{I}, \tilde{\Lambda}, \mathcal{J}, \rho) \mapsto \hat{\lambda}$

WHY IS TUNING SO HARD?

- Tuning is usually **black box**: No derivatives of the objective are available. We can only eval the performance for a given HPC via a computer program (CV of learner on data).
- Every evaluation can require multiple train and predict steps, hence it's **expensive**.
- Even worse: the answer we get from that evaluation is **not exact, but stochastic** in most settings, as we use resampling.
- **Categorical and dependent hyperparameters** aggravate our difficulties: the space of hyperparameters we optimize over can have non-metric, complicated structure.
- Many standard optimization algorithms cannot handle these properties.

