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) $\boldsymbol{\lambda} \in \tilde{\boldsymbol{\Lambda}}$ for an learner $\mathcal{I}_{\boldsymbol{\lambda}}$.

OBJECTIVE AND SEARCH SPACE

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

$$\tilde{\Lambda} = \tilde{\Lambda}_1 \times \tilde{\Lambda}_2 \times \dots \times \tilde{\Lambda}_l$$

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:

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

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

OBJECTIVE AND SEARCH SPACE

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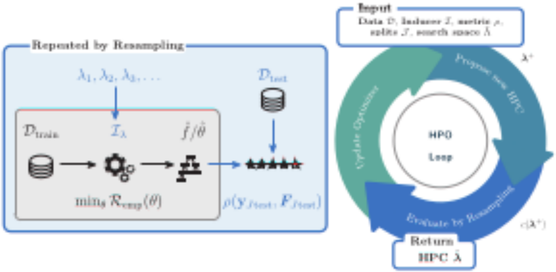

- Evals are stored in **archive** $\mathcal{A} = ((\boldsymbol{\lambda}^{(1)}, c(\boldsymbol{\lambda}^{(1)})), (\boldsymbol{\lambda}^{(2)}, c(\boldsymbol{\lambda}^{(2)})), \dots)$, with $\mathcal{A}^{[t+1]} = \mathcal{A}^{[t]} \cup (\boldsymbol{\lambda}^+, c(\boldsymbol{\lambda}^+))$.
- We can define tuner as function $\tau : (\mathcal{D}, \mathcal{I}, \tilde{\boldsymbol{\Lambda}}, \mathcal{J}, \rho) \mapsto \hat{\boldsymbol{\lambda}}$