Optimizing Discrete Spaces via Expensive Evaluations: A Learning to Search Framework

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Problem Setup and Key Challenge

- **Problem**: Optimize discrete spaces (e.g., sets, sequences, graphs) via expensive black-box function evaluations
  - Multi-core chip design via simulations; Materials design via physical lab experiments

- **Bayesian Optimization (BO) Framework**

$$\text{Statistical model } (\mathcal{M})$$

$$\text{Acquisition Function Optimization (AFO)}$$

$$\max_{x \in X} \mathcal{A}(\mathcal{M}, x)$$

Hard non-linear combinatorial optimization problem with constraints!
Key Idea: Integrate combinatorial search with machine learning methods to solve AFO problems

Repeatedly execute the following two steps

Step 1: Execute search strategy $\mathcal{A}$ guided by current search control knowledge $\mathcal{H}$ to uncover promising structures

Step 2: Update the parameters of $\mathcal{H}$ using the online training data generated from the past search experience