Adaptive Kernel Design for Bayesian Optimization Is a Piece of CAKE 🍰 with LLMs

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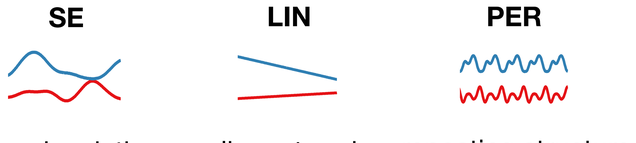
NEURAL INFORMATION PROCESSING SYSTEMS

TL;DR We introduce an **adaptive kernel design** method that leverages **LLMs as genetic operators** to evolve Gaussian process (GP) kernels during Bayesian optimization (BO)

Motivation

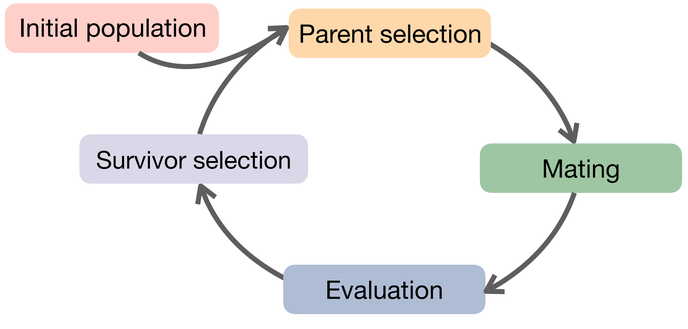
The efficiency of BO depends on the choice of the GP kernel



⚠️ A poor kernel choice can lead to **biased exploration**, **slow convergence**, and **suboptimal solutions**!

Context-Aware Kernel Evolution (CAKE) 🍰

Reframe kernel design problem as an **evolutionary process**:

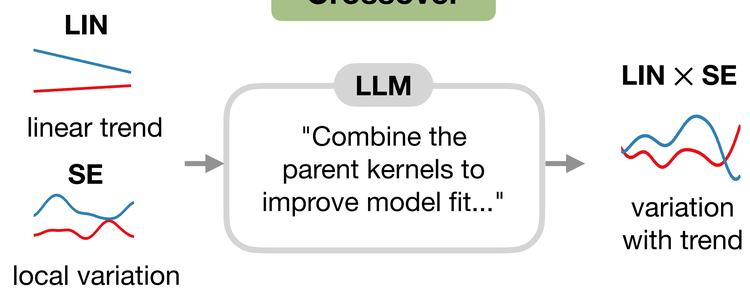


BIC-Acquisition Kernel Ranking (BAKER) 👨‍🍳

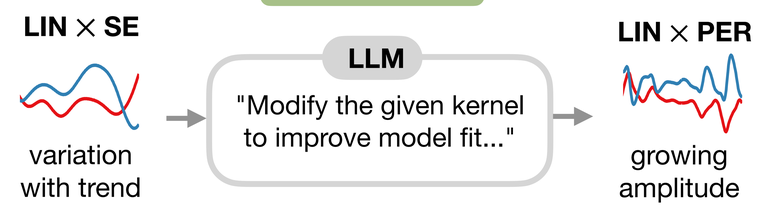
Select the best kernel at each step by jointly optimizing:

1. How well the kernel **explains** the observed data
2. How **promising** the kernel's proposed next query point is

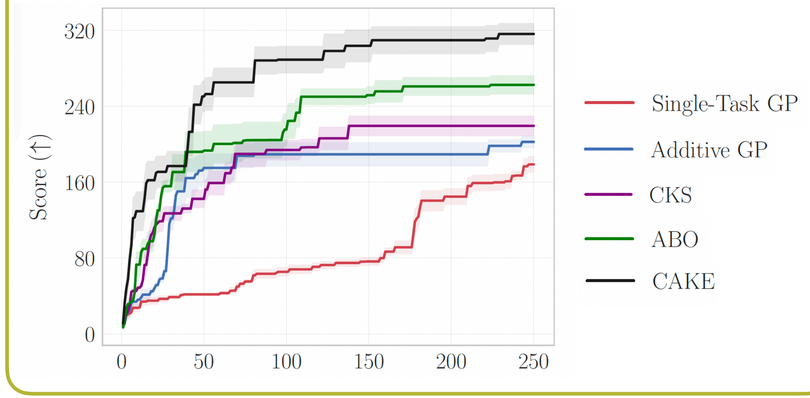
Crossover



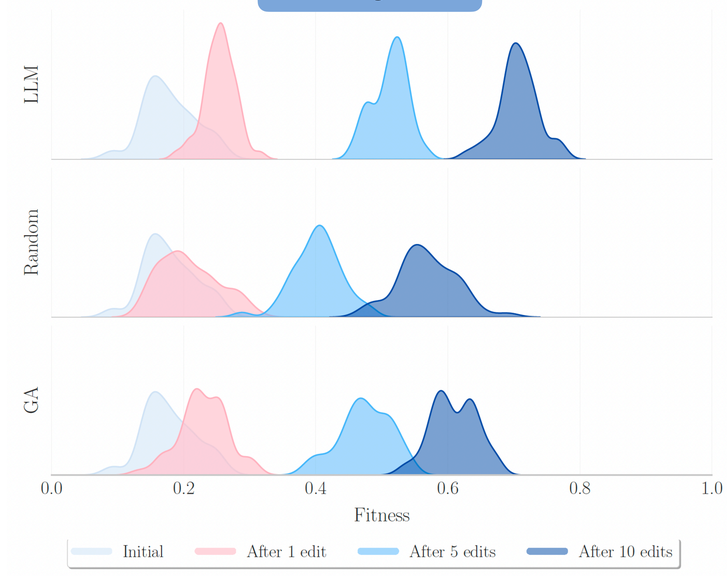
Mutation



Photonic Chip Design



Analysis



LLM-guided evolution achieves **faster convergence** and **higher population fitness** over time

Hyperparameter Optimization