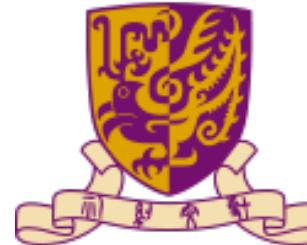


NEURAL INFORMATION  
PROCESSING SYSTEMS

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

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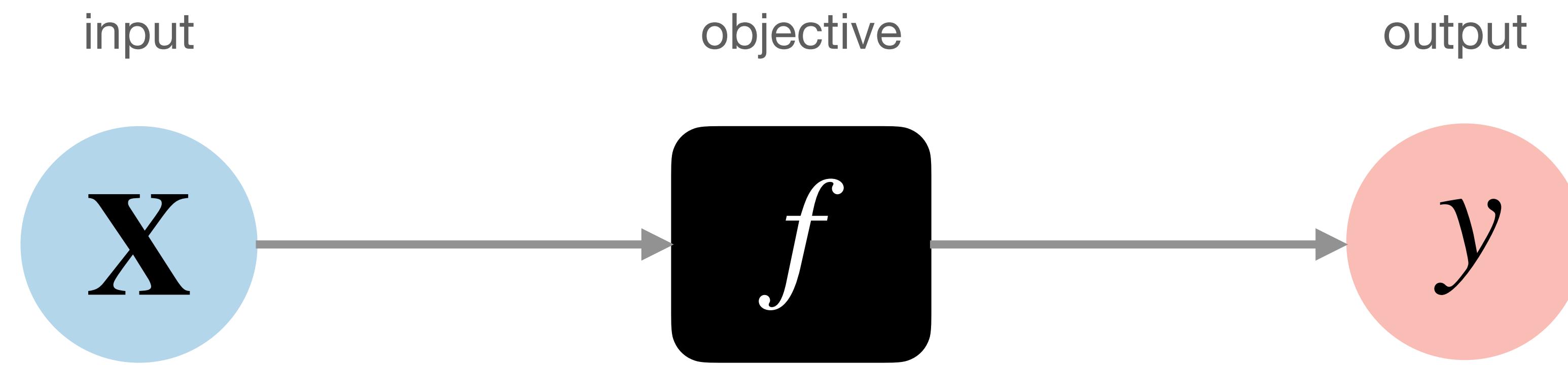
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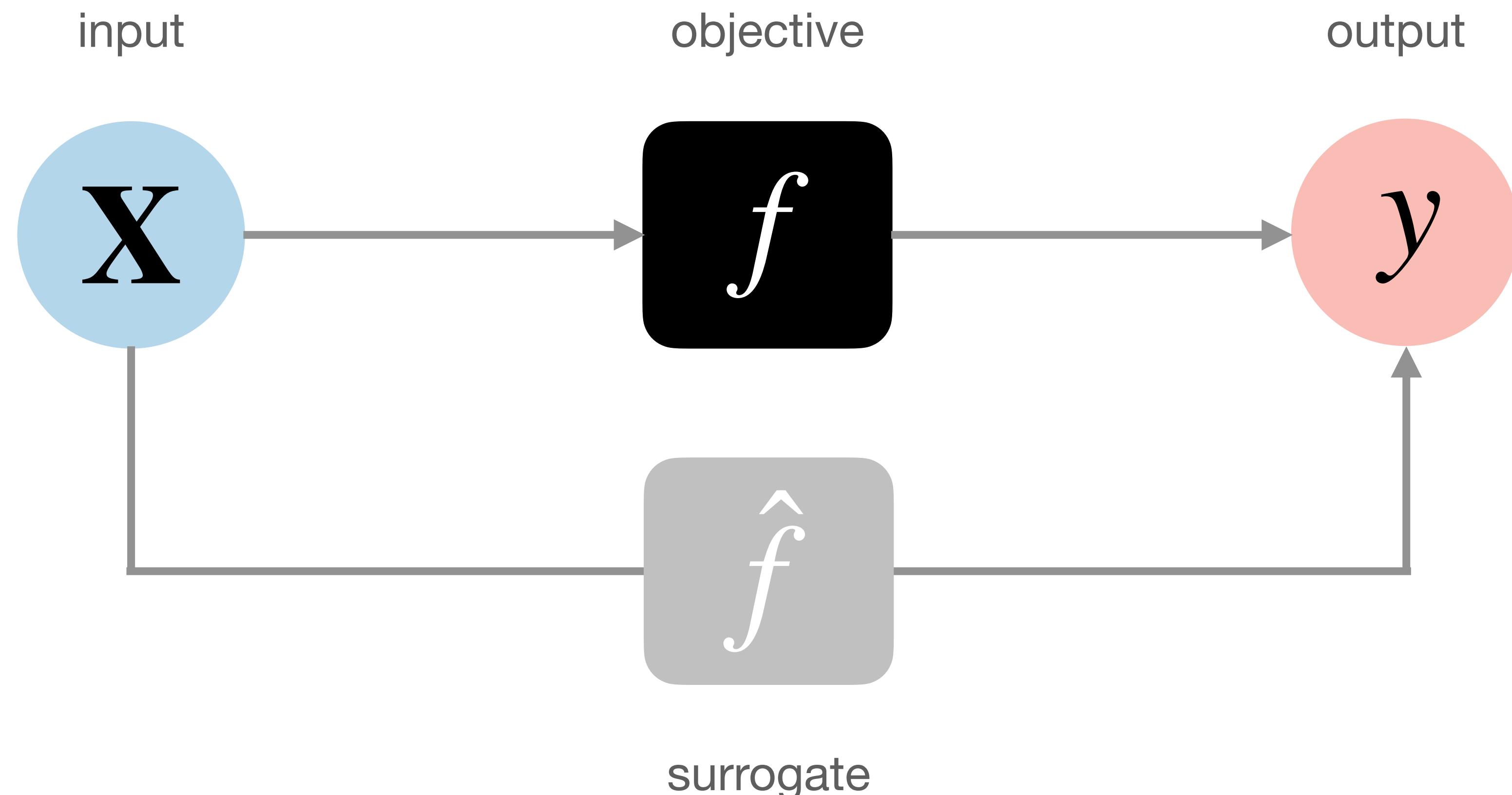
# Black-box optimization

Consider a **black-box** objective that is **expensive-to-evaluate**



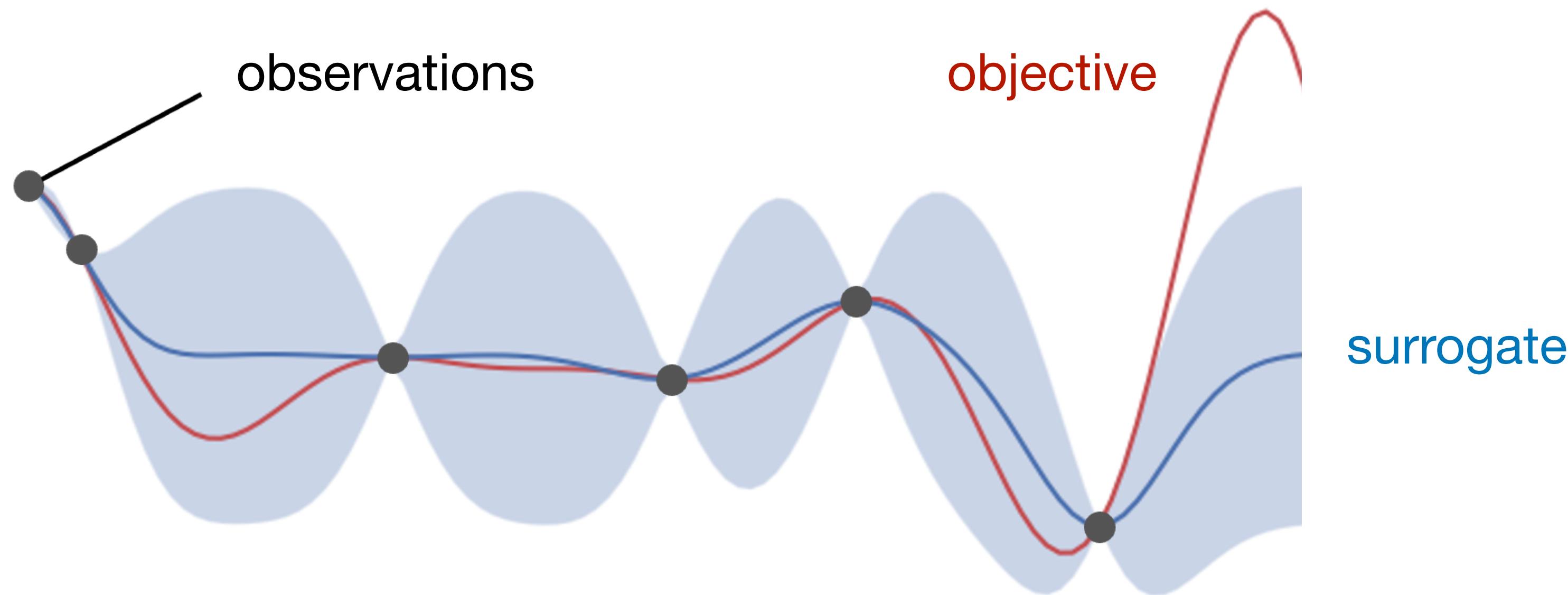
# Black-box optimization

Estimate the objective with a **surrogate**



# Bayesian optimization

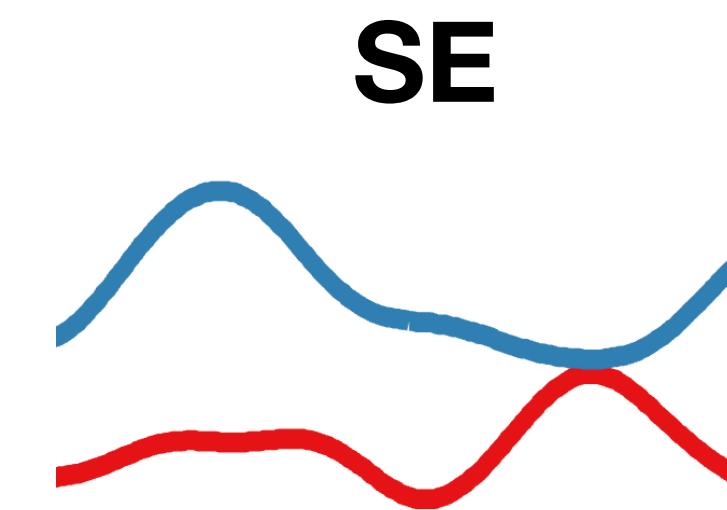
Use a **Gaussian process (GP)** surrogate:  $\hat{f} \sim \mathcal{N}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$



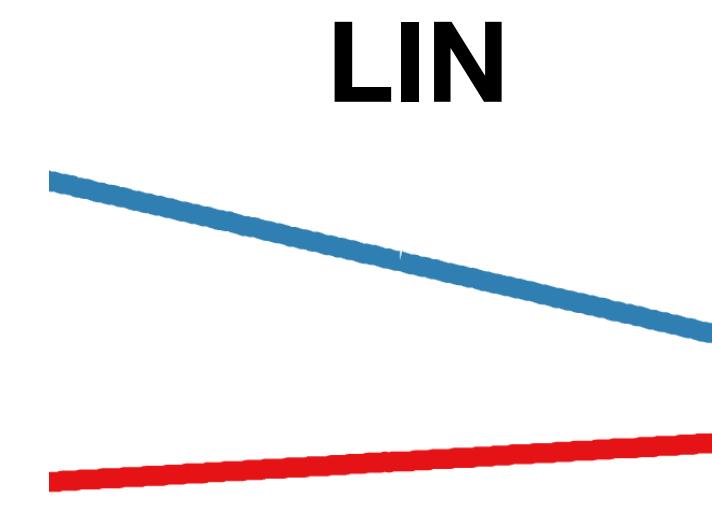
The behavior of a GP *heavily* depends on the **kernel choice**

# Kernel design problem

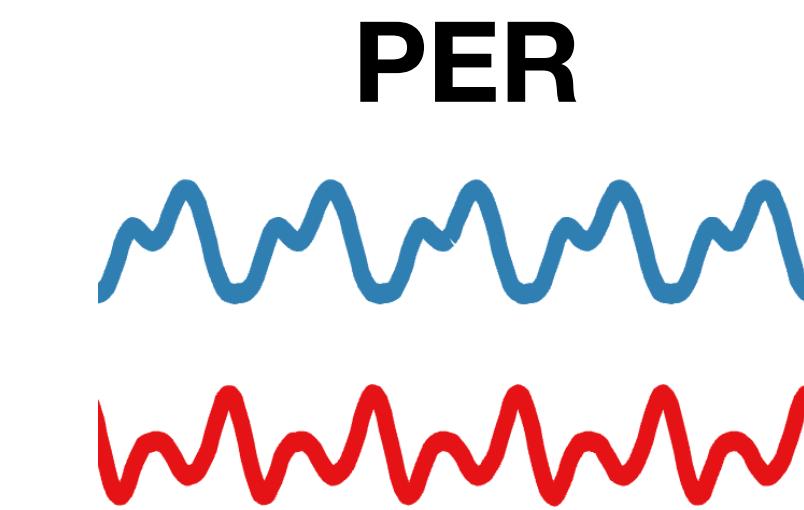
- Different kernel encodes *different assumptions*:



local variation



linear trend



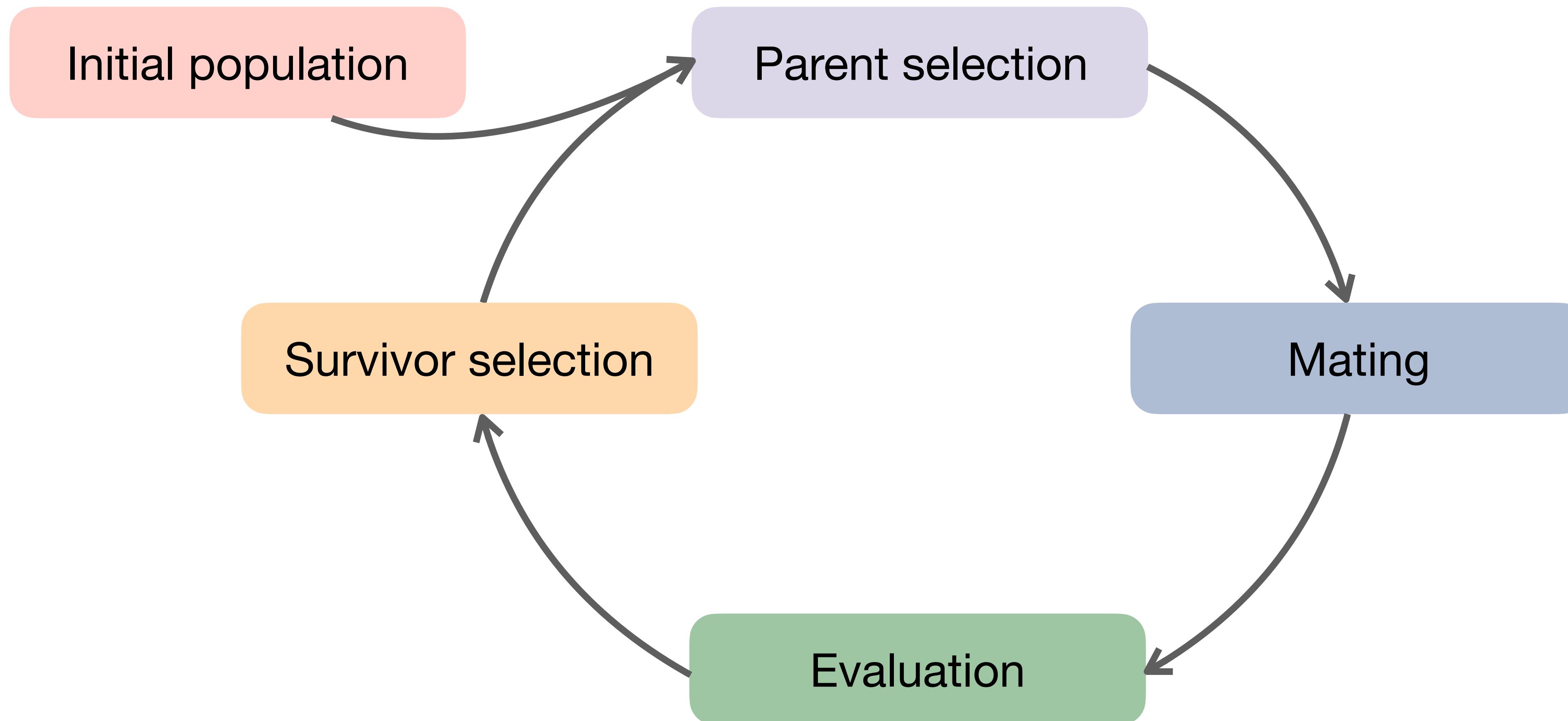
repeating structure

- A poor kernel choice can **hinder convergence**

Which kernel should we use given a problem?

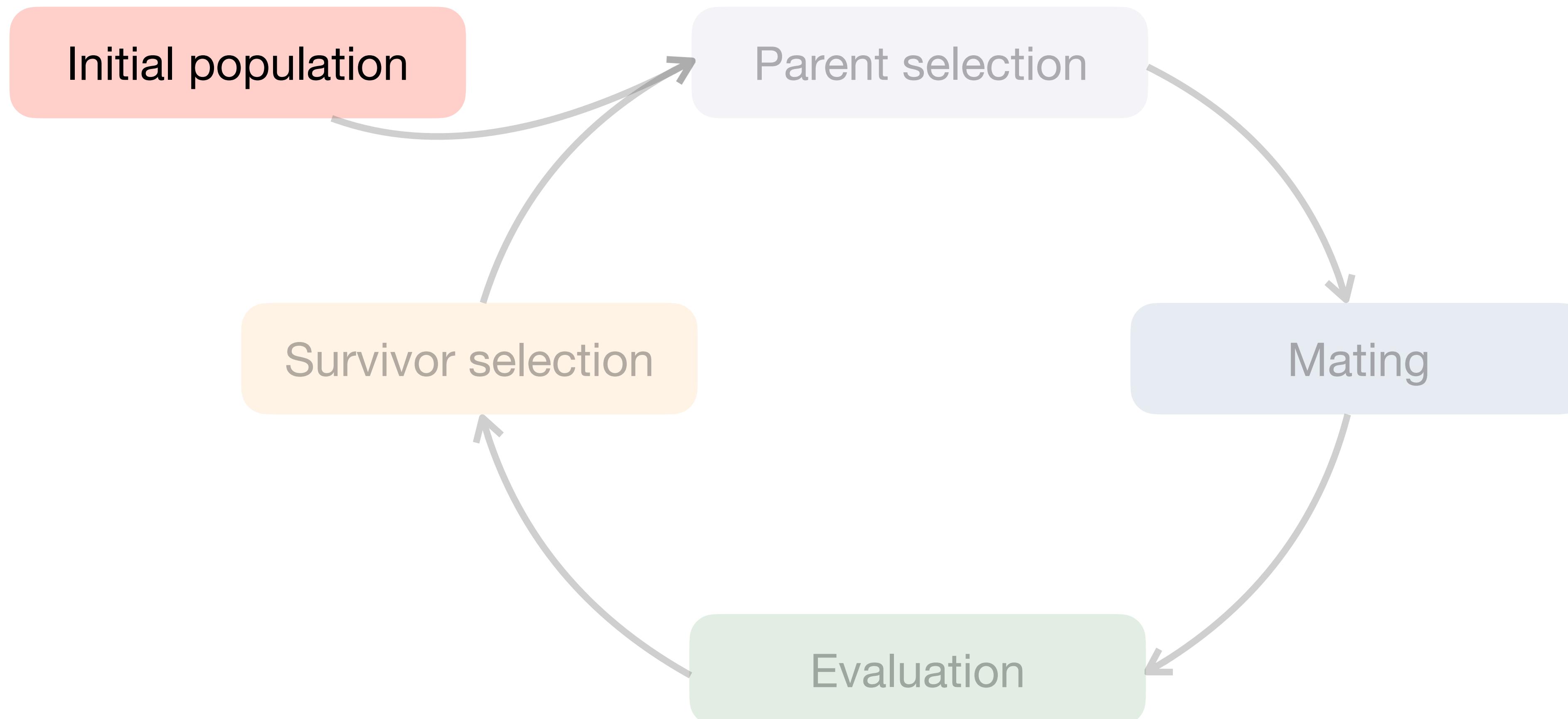
# Context-Aware Kernel Evolution (CAKE)

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



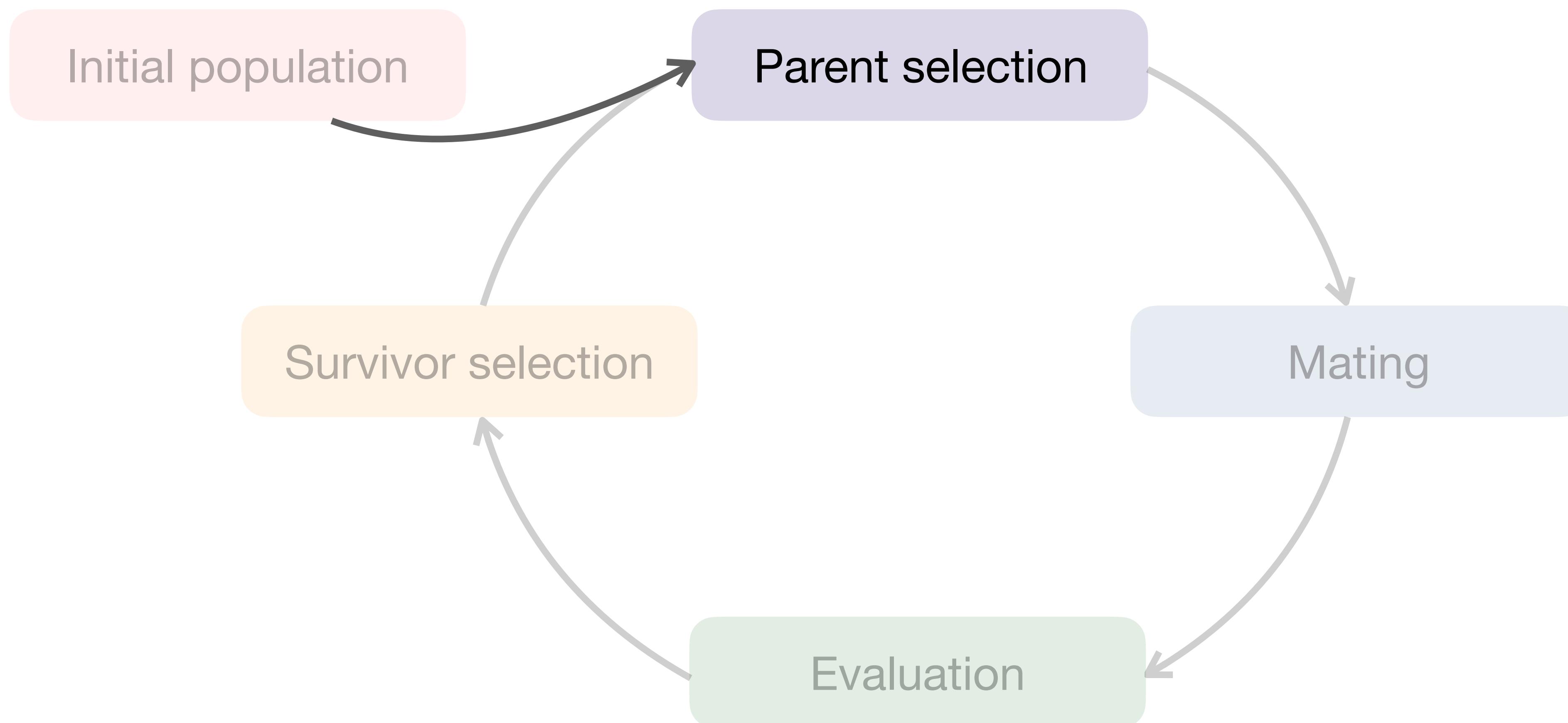
# Context-Aware Kernel Evolution (CAKE)

Start with a set of **base kernels**  $\mathbb{K} = \{\text{SE}, \text{LIN}, \text{PER}, \text{RQ}\}$



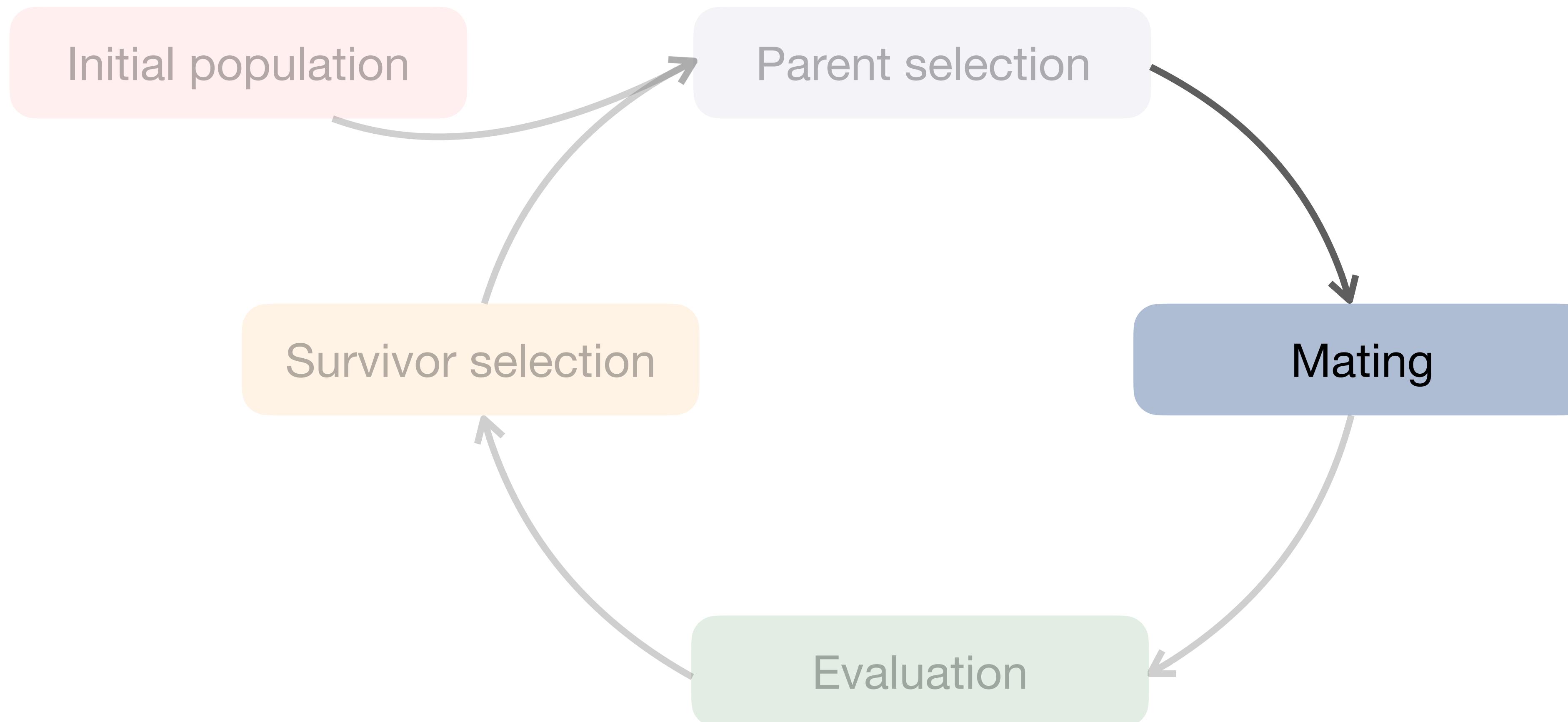
# Context-Aware Kernel Evolution (CAKE)

Sample **parent kernels**  $k_1, k_2$  from the population  $\mathbb{K}$



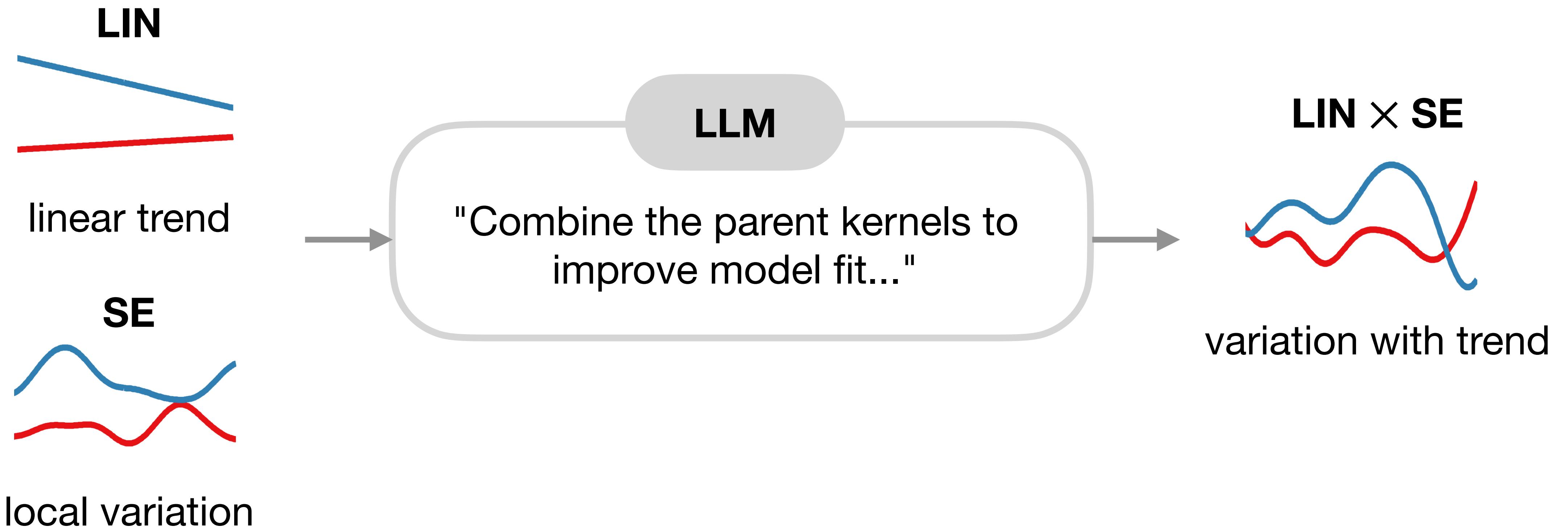
# Context-Aware Kernel Evolution (CAKE)

Generate **new kernels** using LLM as genetic operator



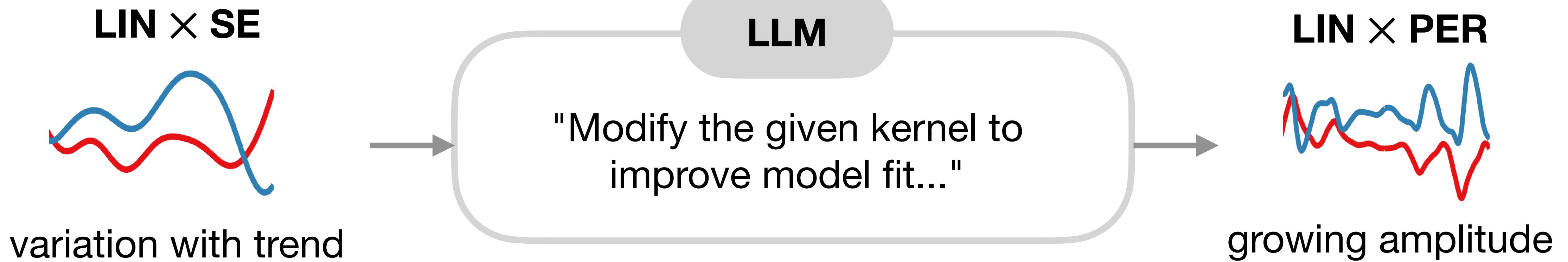
# Mating

Perform **crossover** to generate new offspring kernel



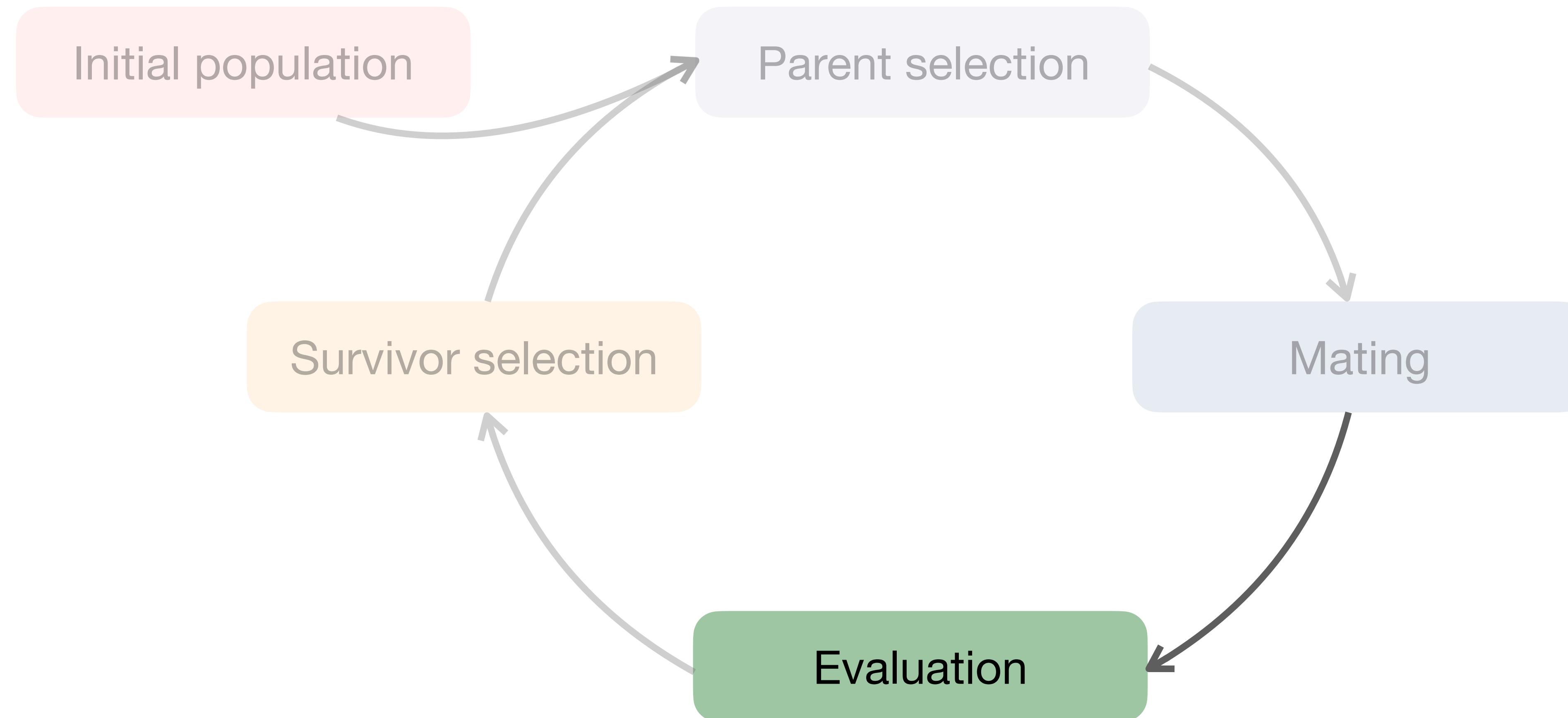
# Mating

Perform **mutation** to refine the kernel



# Context-Aware Kernel Evolution (CAKE)

Measure the **fitness scores** of each kernel in the population



# Evaluation

Measure fitness using the normalized **Bayesian information criterion (BIC)**:

$$\text{fitness}_k = \frac{\exp(-\text{BIC}_k)}{\sum_{k'} \exp(-\text{BIC}_{k'})}$$

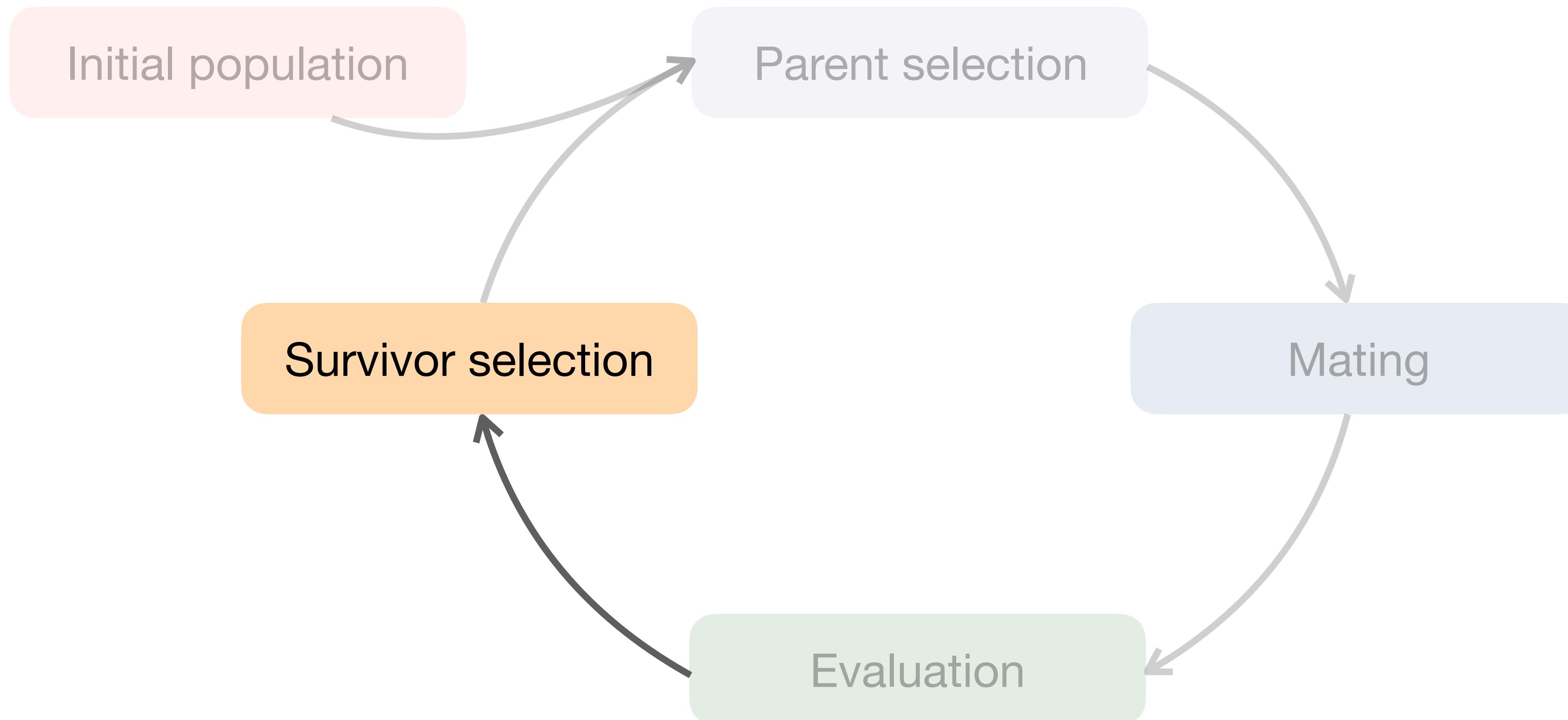
where

$$\text{BIC}_k = -2 \log L_k + p_k \log n$$

model fit                    model complexity

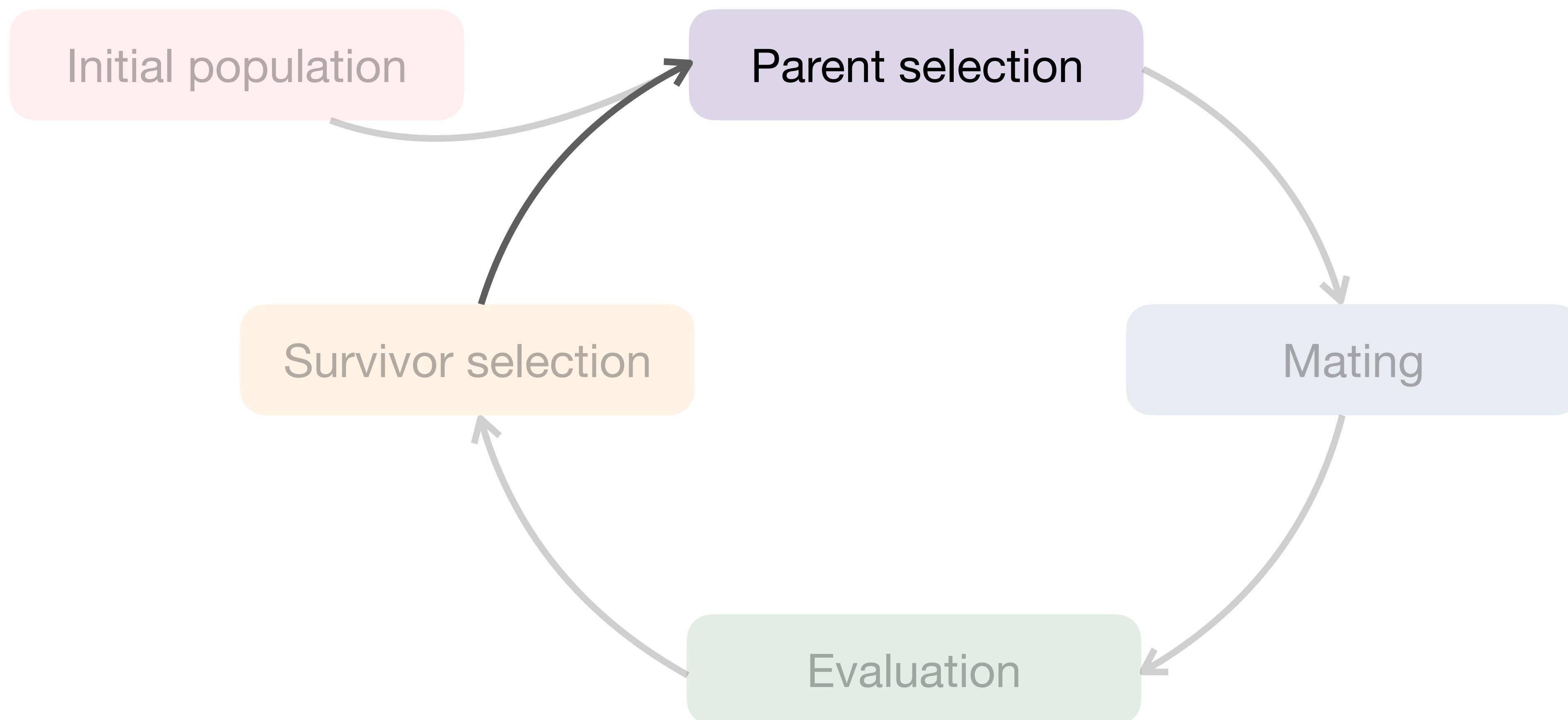
# Context-Aware Kernel Evolution (CAKE)

Select the **top performing kernels** for the next generation

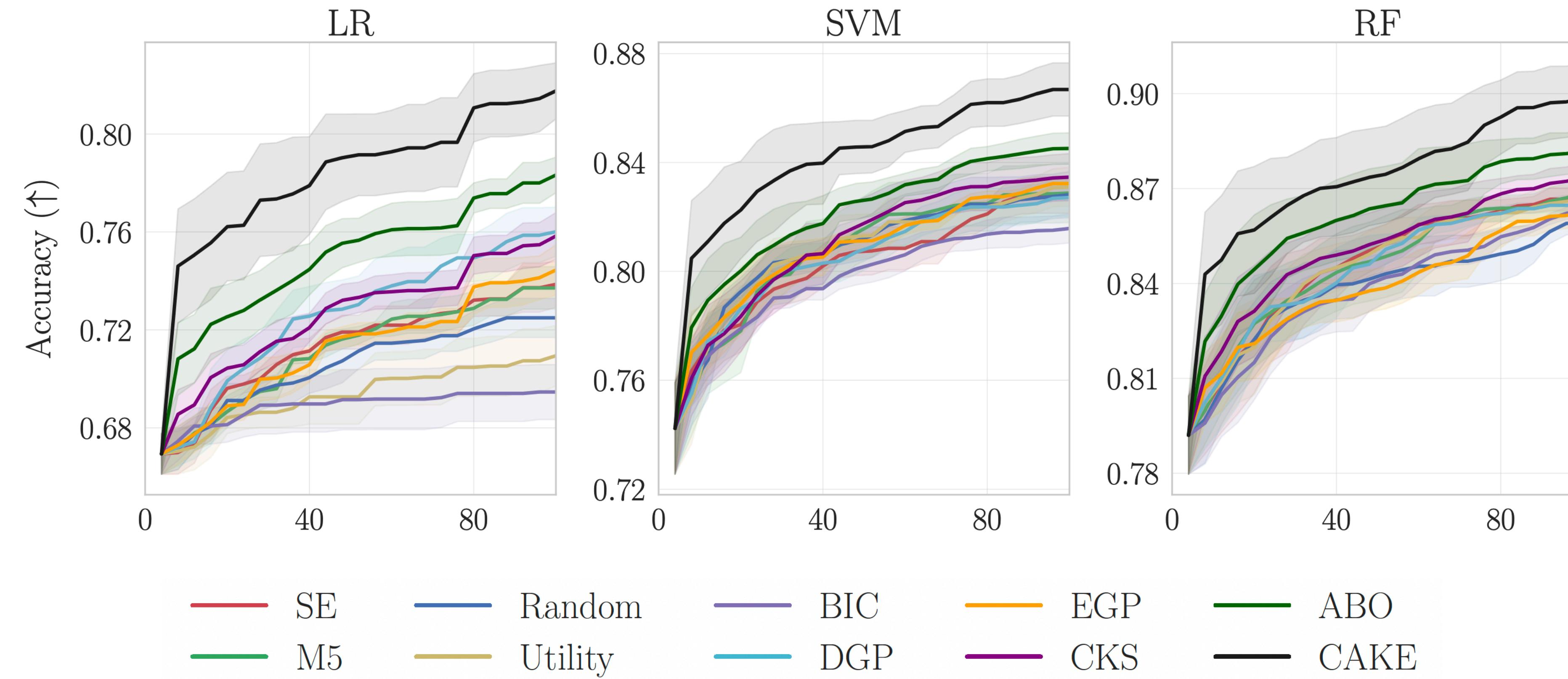


# Context-Aware Kernel Evolution (CAKE)

Repeat until budget is exhausted

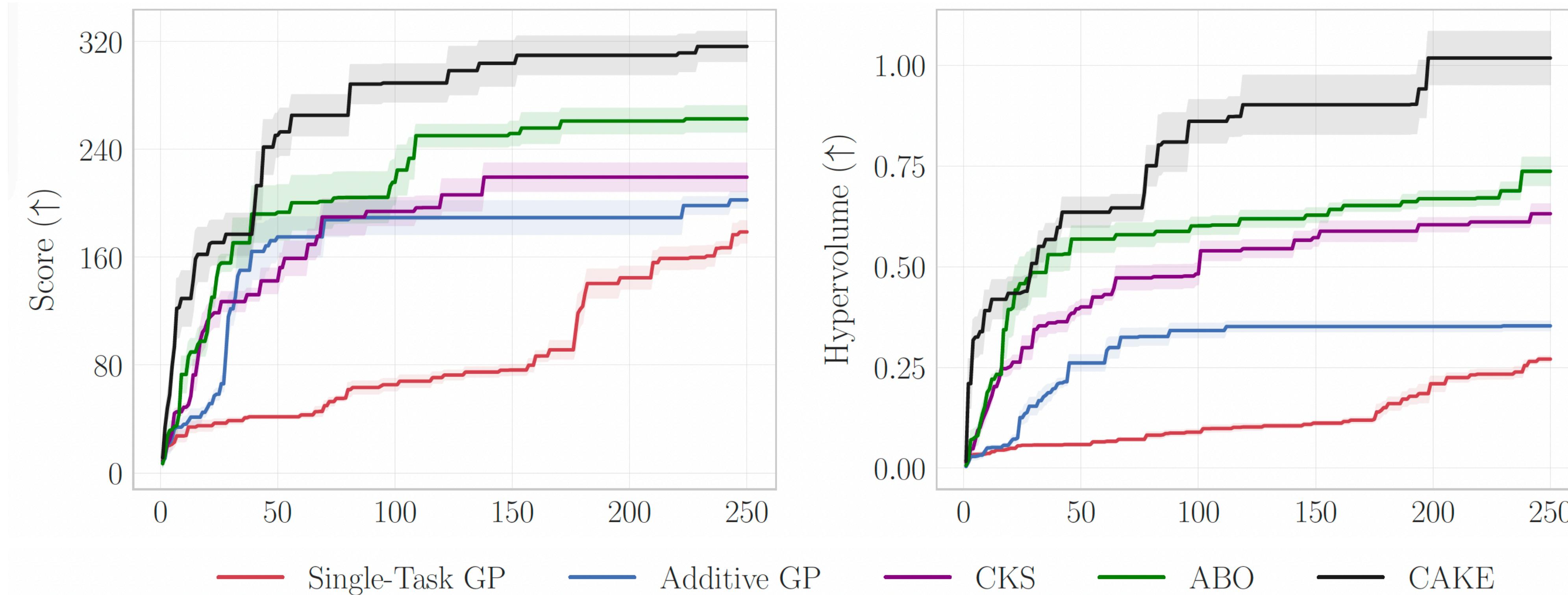


# Hyperparameter optimization



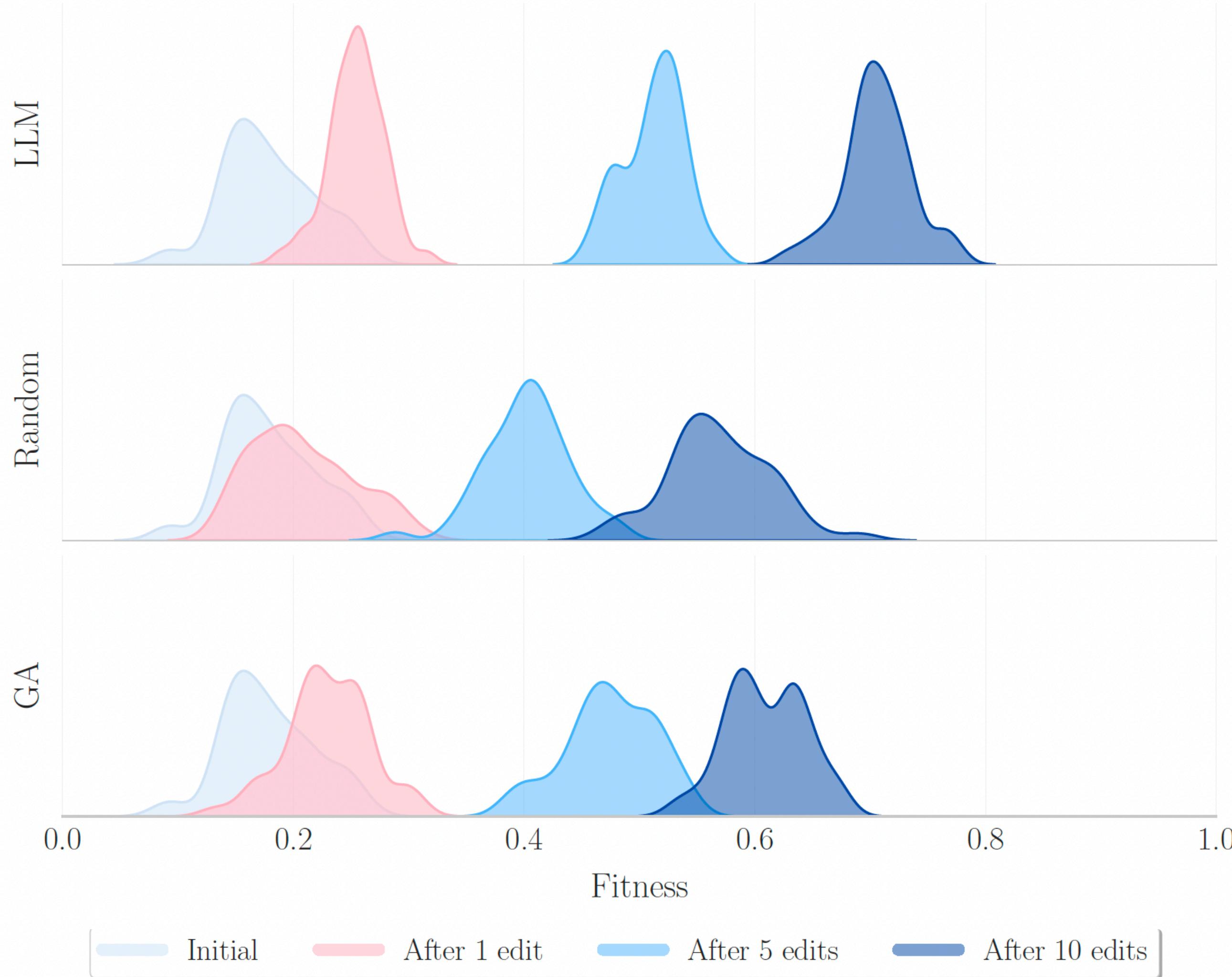
- Consistently achieved **highest test accuracy** on average
- Showed 67.5% of total improvement **within just 25% of the budget**

# Photonic chip design



- Effectively **balanced trade-offs** between objectives
- Demonstrated **10× speedup** in finding high-quality solutions

# Analysis



- After just 1 LLM edit, the distribution immediately shifts toward **higher values**
- LLM edits achieve **faster convergence** and **higher fitness** over time

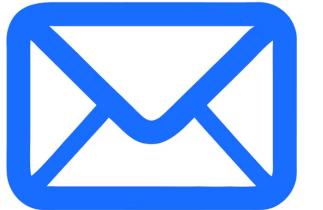
# Thanks for listening!



<https://arxiv.org/abs/2509.17998>



<https://github.com/richardcsuwandi/cake>



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