

PI is back! Switching Acquisition Functions in Bayesian Optimization

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1 TL;DR

- BO's components can be reconfigured at each iteration
- For example, acquisition function (AF) schedules (PI, EI) beneficial
- Showcases potential of dynamic schedules in BO
- Even a simple schedule leads to efficiency improvements

2 Motivation + Method

Motivation

- BO has several key design components, incl. surrogate model, acquisition function (AF), initial design
- Online schedules of AFs beneficial [Portfolio Allocation, Hoffmann et al., 2011; Dragonfly, Kandasamy et al., 2020]
- Dynamic hyperparameter (HP) schedules can be beneficial for iterative algorithms [Karafotias et al., 2015; Doerr & Doerr, 2020; Biedenkapp et al., 2020; Speck et al., 2021, Adriaensen et al., 2022]

Goal Improve sample efficiency of BO

Idea

Dynamically set BO's HPs/components

Method

Switch acquisition functions: EI to PI, make it simple!

Why EI and PI?

EI more explorative, PI more exploitative

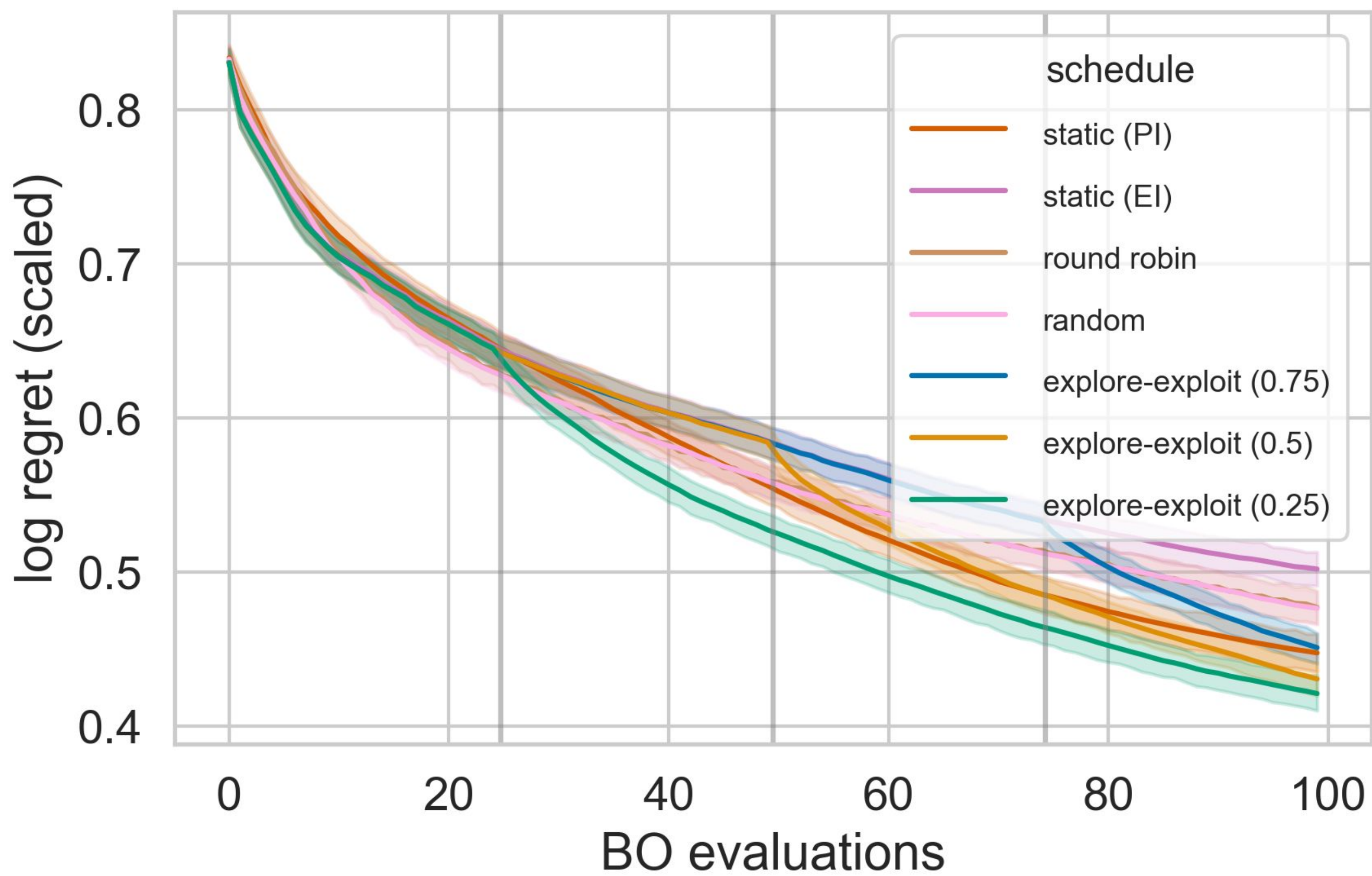
3 Experimental Setup

- 24 BBOB functions of COCO benchmark [Hansen et al., 2021]
- 60 seeds, 5 dimensions, 7 schedules

Name	Schedule
static (EI)	EI EI EI EI
static (PI)	PI PI PI PI
random	EI PI PI EI EI EI PI EI
round robin	EI PI EI PI EI PI EI PI
explore-exploit (0.25)	EI PI PI PI
explore-exploit (0.5)	EI EI PI PI
explore-exploit (0.75)	EI EI EI PI

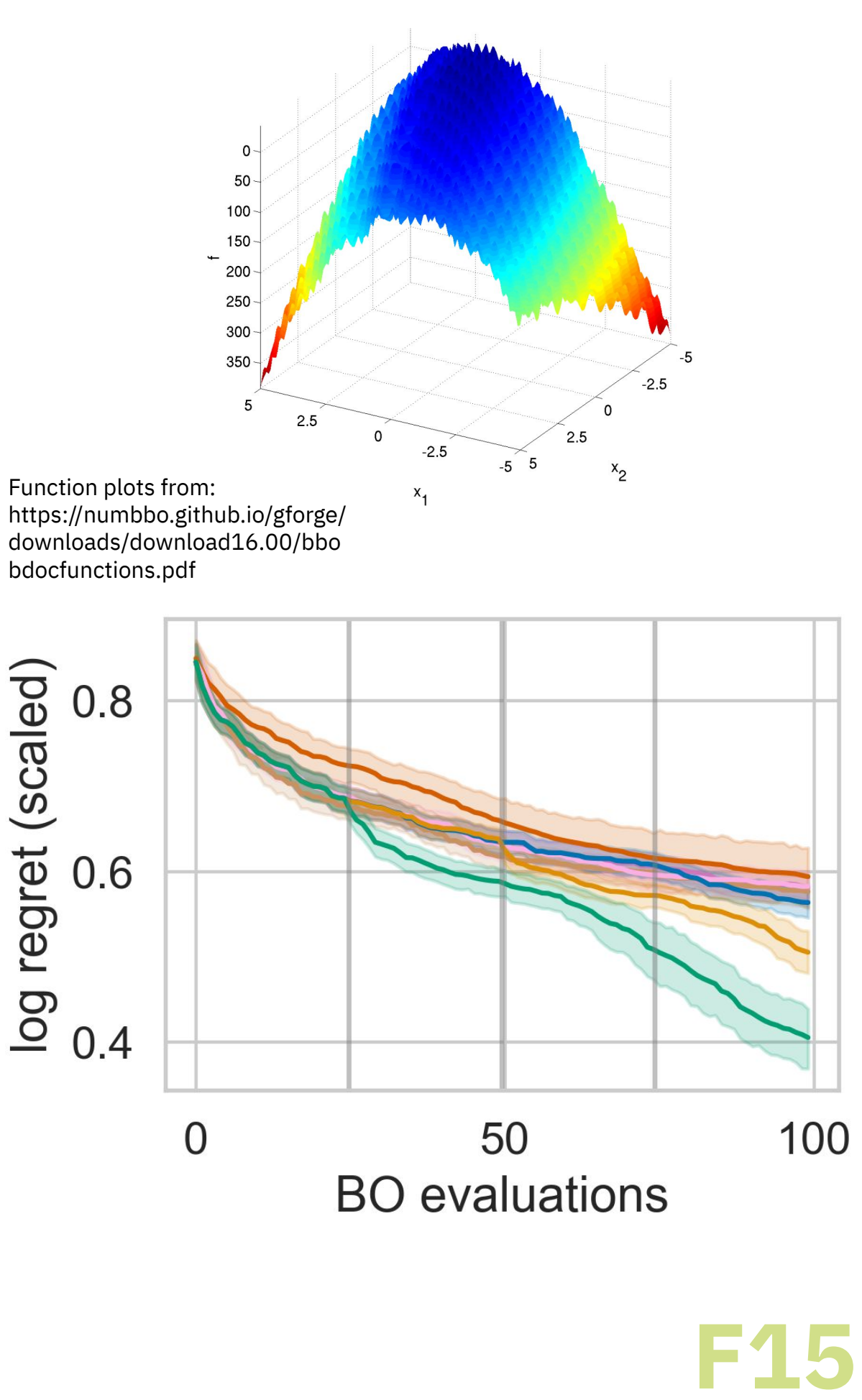
4 Key Insights

Scaled log-regret averaged over all 24 BBOB functions for 5 dims with the 95% CI

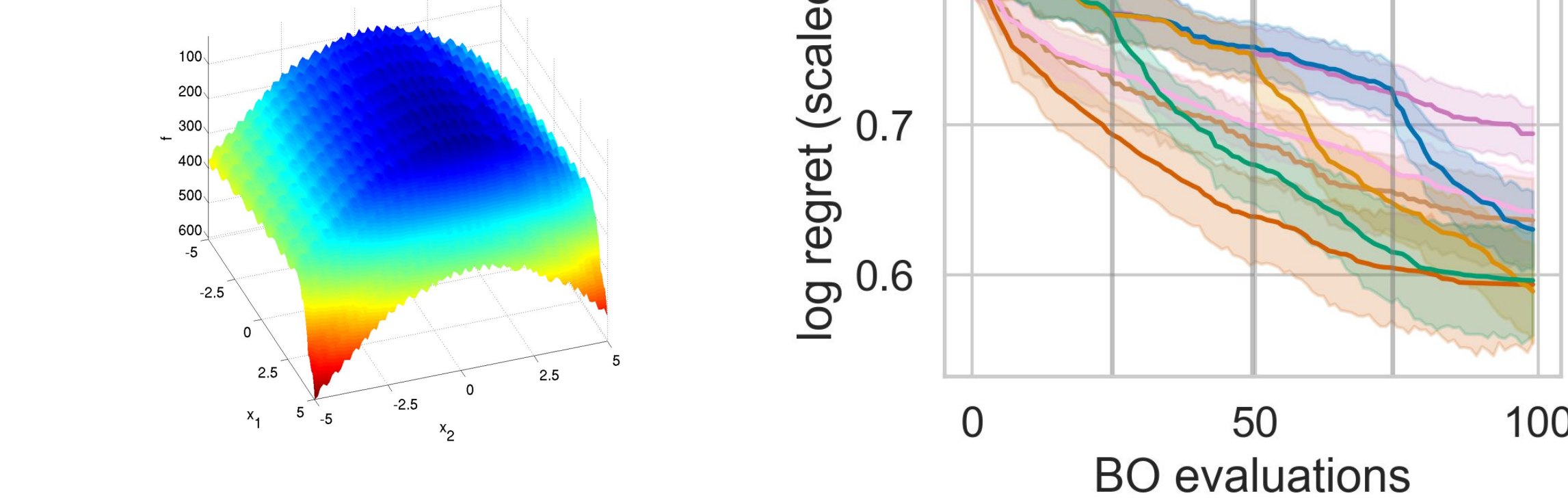


- Optimal choice of AF schedule depends on problem
- Most robust choice: Switch after 25% from EI to PI
- Round-robin \approx random schedule, never best

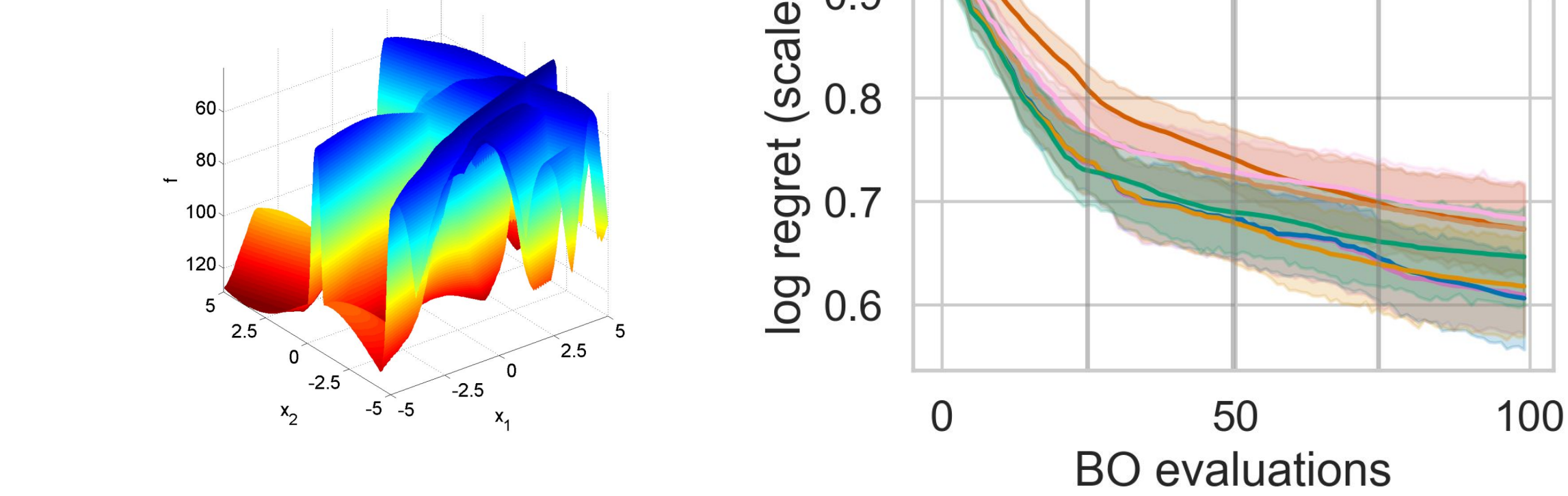
Good global structure?
→ Switch



Uni-model, smooth?
→ Schedule with PI



Multi-modal, weak global structure?
→ Schedule with EI



5 Future Works

- Scale: more dimensions, AFs, schedules, benchmarks
- Meta-learning: learn recommendations for which AF schedule to use
 - based on Exploratory Landscape Analysis (ELA) [Mersmann et al., 2011] features of the initial design → see our poster at the MetaLearn workshop!
- Online selection or learn AF schedules, e.g. via Reinforcement Learning
 - What are good state features of BO?

