

Pareto Front Guided Sampling for Operator-in-the-Loop real time optimization of Chemical Processes

Samuel Stricker,
Dr. Antonio Del Rio Chanona,
Dr. Mehmet Mercangöz

Motivation

- Optimization in chemical systems can be expensive, gradient-free, and uncertainty-dominated [1].
- Classical BO performs well but offers limited interpretability.
- Expert priors (feasible regions, safety intuition) are rarely incorporated.

Pareto Front Guided Sampling

- Bayesian Optimization based DoE Algorithm for multi-objective optimization [2].
- Constructs Pareto fronts from surrogate model's predicted means and uncertainties.
- Explicit visualization of exploration-exploitation structure and constraint trade-offs:
 - Objectives:** maximization of mean value
 - Exploration:** maximization of uncertainty
 - Constraints:** probabilities of satisfying the constraint
- Enables expert-driven selection and systematic exclusion of unsafe or low-value regions.

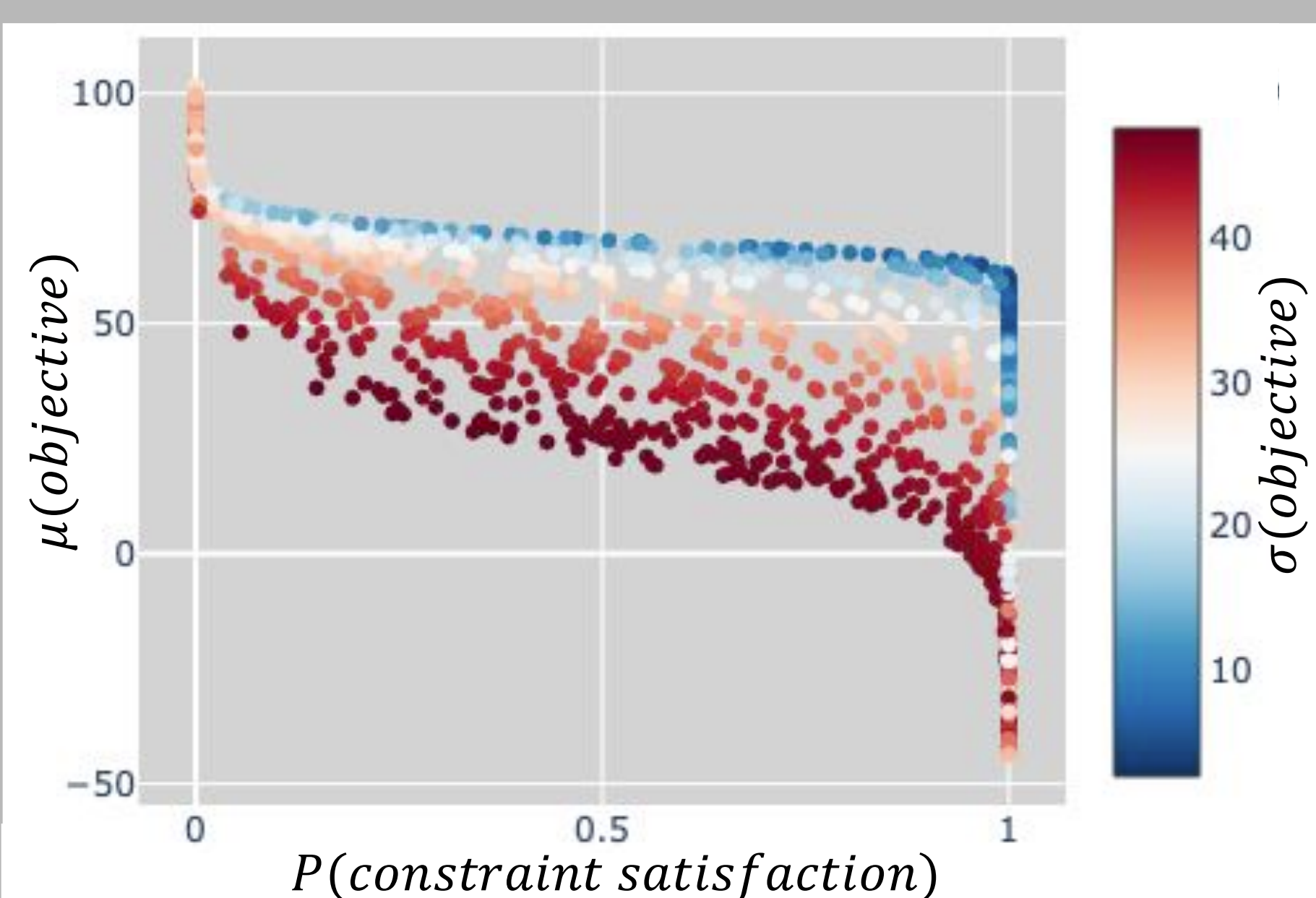


Figure 1 Example of a pareto front where x axis is a probability of satisfying a given constraint, y axis is the maximization of the mean objective value (exploitation) and the color represents the uncertainty of the objective (exploitation)

Case Study: Non-isothermal CSTR

- Nonlinear, exothermic parallel reactions with strict safety bound (Temperature < 540 K).
- Desired product B is produced using A and D, while A reacts with itself to undesired product C.

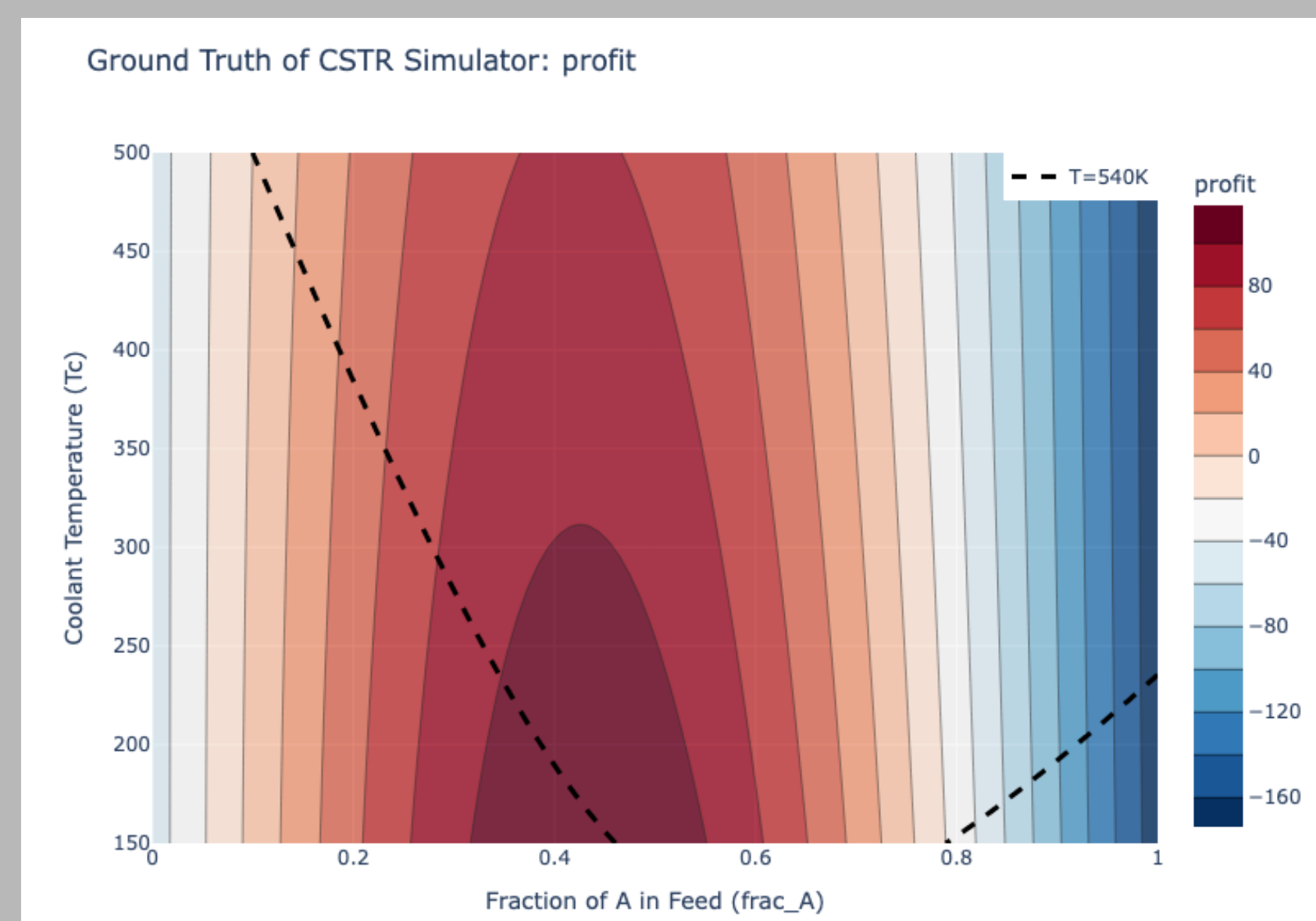
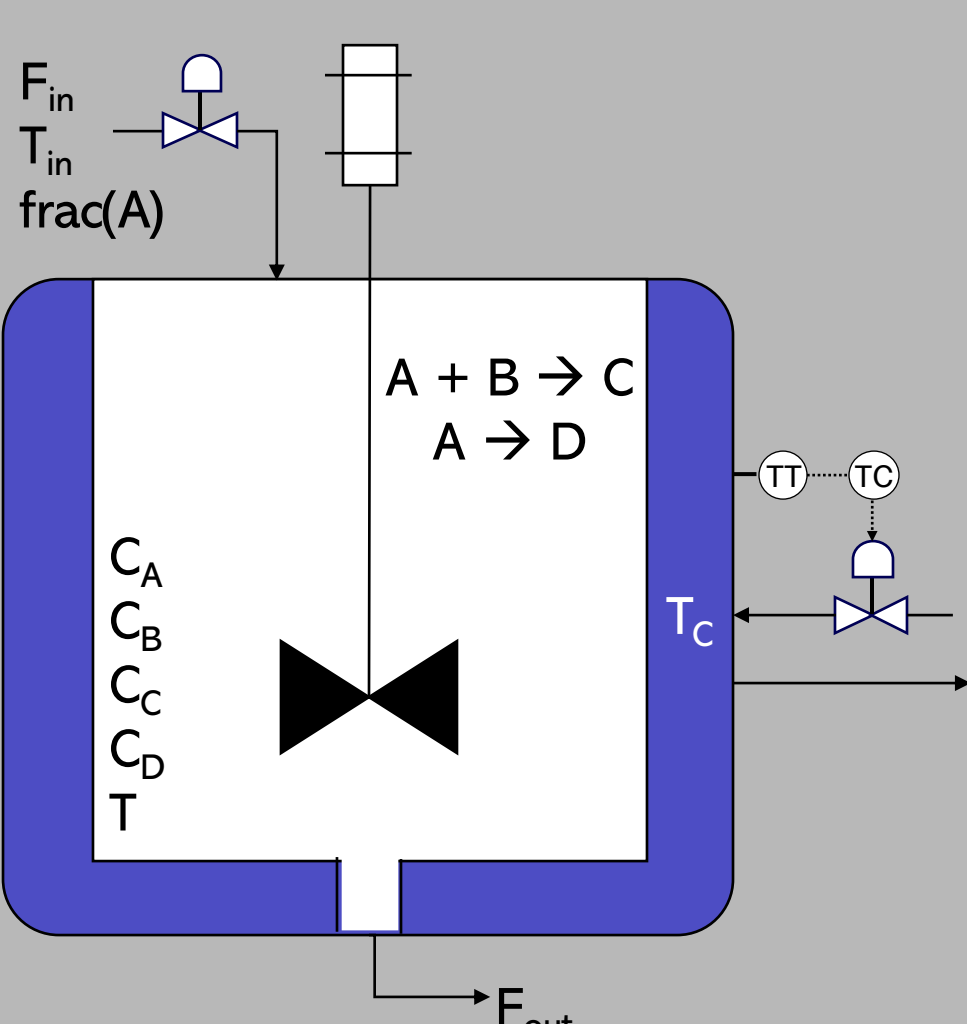


Figure 2 (left) scheme of CSTR reactor and reactions. (right) profit landscape as a function of fraction of A (frac(A)) in feed and cooling temperature (T_c).

Methods

- Training of 5 Gaussian Process regressors for concentrations of A, B, C, D and temperature T .
- Create Pareto Front using NSGA-II algorithm using the following optimization axis:
 - Probability of $T < 540 K$ (maximization)
 - Mean predicted Profit (maximization)
 - Standard Deviation of predicted Profit (maximization)
- Exclusion of undesired experiments (automated):
 - $P(T < 540) > 0.8$
 - $\mu(\text{Profit}) > \max(\text{Profit}(\text{Experiments}))$
 - If possible: $\sigma(\text{Profit}) > 0.25 * \max(\sigma(\text{Profit}))$
- Sample experiment with min minimum L2 distance to Utopia Point (best of value of each objective)

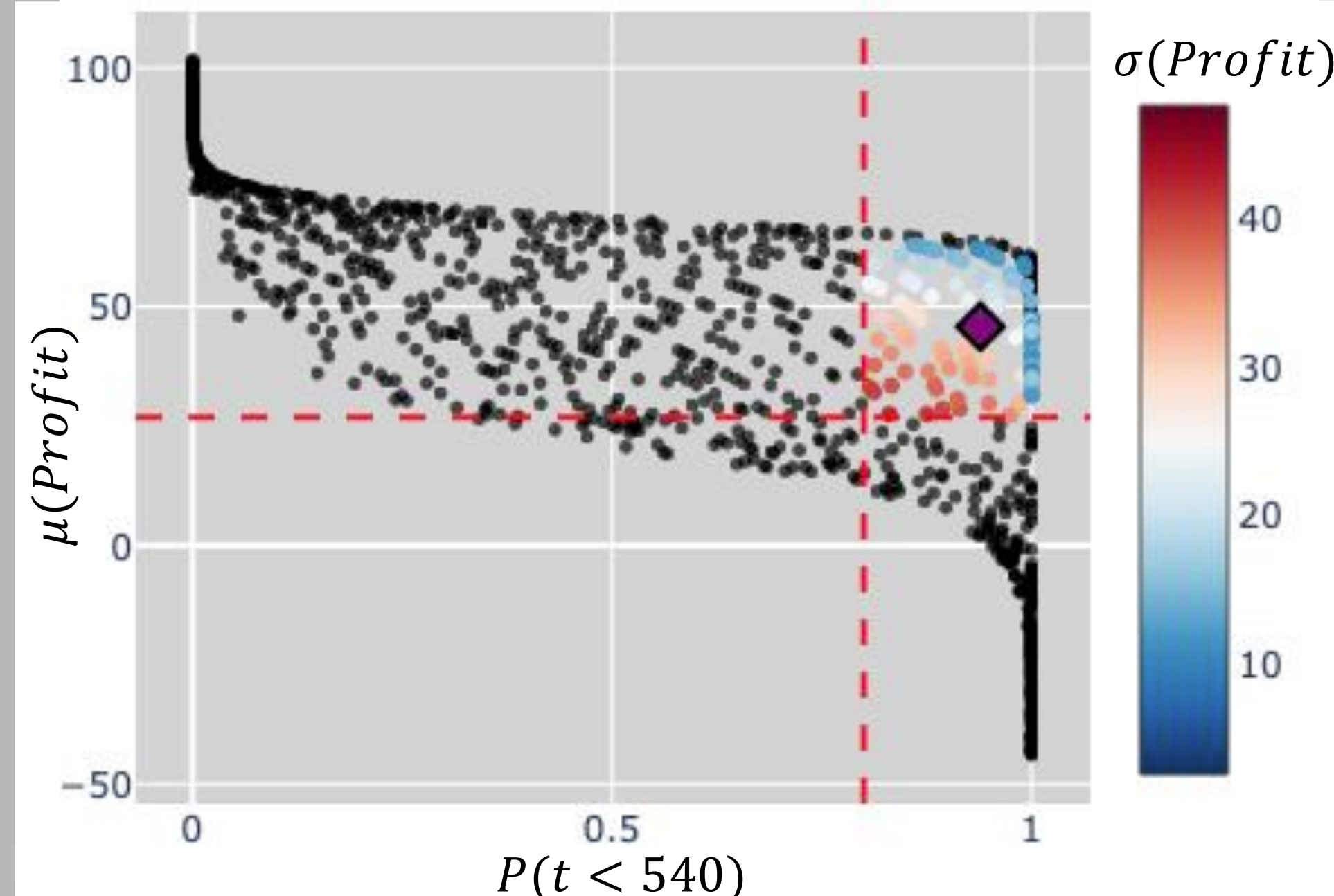


Figure 3 Pareto front with excluded regions (black). From the remaining potential experiments (colored) the closest to the utopia point (1, 62, 42) is selected (violet).

Results & Discussion

- Four start points on left/right side of constraint barrier
- Both converge to optima without any temperature violation
- Algorithm manages to jump the constraint barrier with low risk of constraint violation

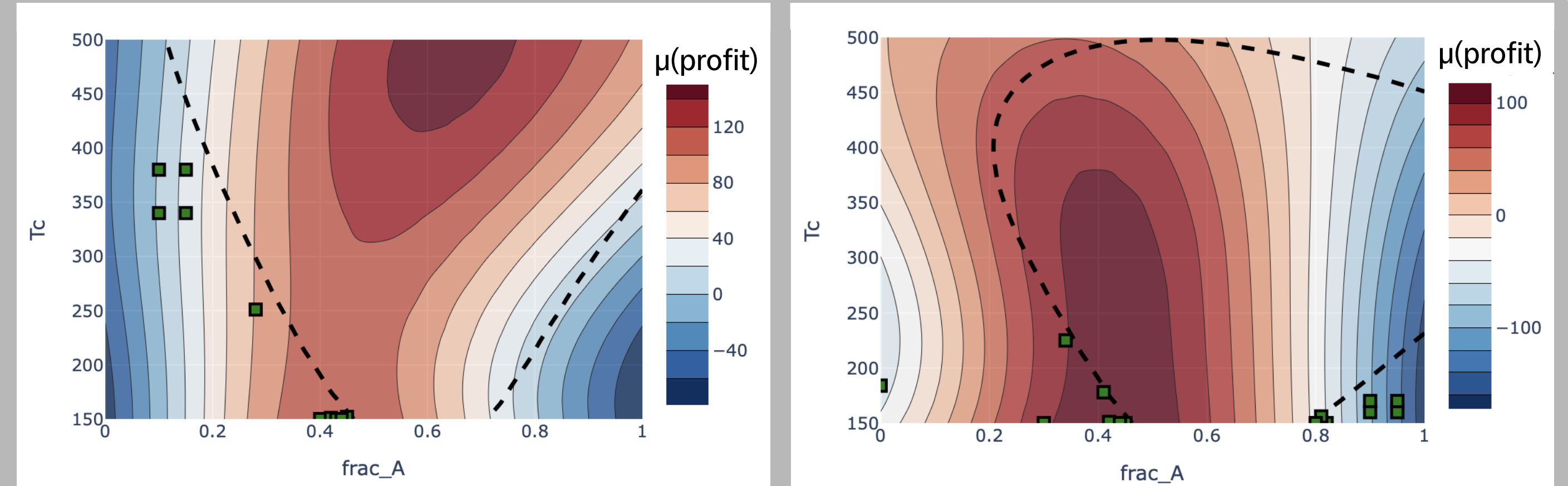


Figure 4 GP's mean profit prediction starting on left- (left) and righthand side (right) of the constraint barrier. Performed experiments are shown in green and the predicted constraint line ($T=540K$) dashed.

Outlook

- Human-in-the-loop: more sample efficient
- Multi-Fidelity optimization: to adhere to cost/time constraints

References

- [1] T. Savage, E. A. d. R. Chanona, Human-Algorithm Collaborative Bayesian Optimization for Engineering Systems, 2024.
- [2] S. Stricker, MSc. Thesis, ETH Zurich, Zurich, 2024.