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TRADEOFF-AWARE BAYESIAN ACTIVE LEARNING WITH VARYING COST FOR FEASIBLE REGION IDENTIFICATION

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ABSTRACT

Understanding design requirements in engineering design, requires identifying regions in the design space that satisfy these constraints. This is called feasible region identification. As running (random) simulations is expensive, a cost- and data-efficient sampling approach is needed to find the feasible designs. Bayesian Active Learning (AL) is an iterative sampling method that uses a surrogate, e.g. a Gaussian process, and an acquisition function to select the next sample. This research focuses on creating new acquisition functions. On the one hand, cost-aware variants are investigated. These acquisition functions incorporate an unknown simulation cost and sample more designs using the same budget while also finding more feasible designs. On the other hand, we look at the exploration-exploitation trade-off of the acquisition function as a two-objective problem which leads to the creation of two acquisition functions based on scalarization methods. The scalarization-based acquisition functions often outperform most state-of-the-art acquisition functions.

1 INTRODUCTION

Early on in the engineering design process, the aim is to understand design constraints and their feasibility before optimizing the design. For a d-dimensional design space with L constraints this becomes the problem $G(\mathbf{x}) = (g_1(\mathbf{x}), \ldots, g_L(\mathbf{x}))^\top \leq (t_1, \ldots, t_L)^\top$, where $g_l : \mathbb{R}^d \to \mathbb{R}$ is the l-th constraint function with threshold t_l. Often G requires expensive simulations. In the case of Feasible Region Identification (FRI) the goal is to understand the feasibility of the problem and to locate feasible designs (Nikova et al. 2022).

Bayesian Active Learning (AL) is a data-efficient iterative sampling approach that can be used for FRI. It uses a surrogate, like a Gaussian process (GP), that provides uncertainty with the prediction. A GP is trained for each g_l independently on data $\mathscr{D}_l$ and serves as a cheap alternative $\hat{G}$ that is used in the acquisition decision. An acquisition function $\alpha(\mathbf{x}, \hat{G}, \mathbf{t})$, which is being optimized at each iteration, drives the sampling. These functions balance a trade-off between exploring the full design space or exploiting the feasible region. The iterations stop when the simulation budget is depleted. This can be a number of samples or a total simulation cost (e.g., time or energy).

The simulation cost can sometimes depend on the design vector $\mathbf{x}$, while the cost function is unknown. This unknown and varying cost can influence the sample preference. Hence, Nikova et al. (2023) extend the *Probability of Feasibility and Variance (PoFV)* acquisition function using two cost-aware strategies.

We follow the perspective of De Ath et al. (2021) to approach the exploration-exploitation trade-off in acquisition functions as a two-objective problem. Nikova et al. (2024) show that this trade-off exists in state-of-the-art acquisition functions, and also create two new acquisition functions based on scalarization methods, i.e., a strategy to solve two-objective problems as a single objective.

2 MAIN CONTRIBUTIONS

The variance (VAR) σ^2 of a prediction given by the GP is often used for exploring the design space and is needed to improve the surrogate performance. Exploiting the design space for feasible regions is

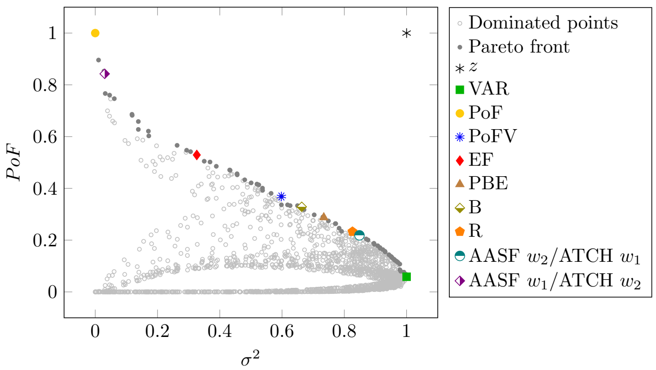

Figure 1: Exploration-exploitation objective space: each acquisition function chooses another sample on the front. AASF and ATCH choice depends on weights. (Nikova et al. 2024)

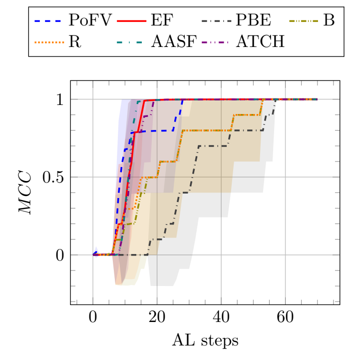

Figure 2: *Matthews Correlation Coefficient (MCC)* of a constraint surrogate: mean and standard deviation of 10 runs.

done with the *Probability of Feasibility (PoF)*: $F(\mathbf{x}) = \prod_{l=1}^{L} p(p(g_l|\mathbf{x}, \mathscr{D}_l) \leq t_l)$. PoFV multiplies these two components: $\alpha_{PoFV} = \prod_{l=1}^{L} p(p(g_l|\mathbf{x}, \mathscr{D}_l) \leq t_l)\sigma_l^2(\mathbf{x})$, and samples inside the feasible region. Note that other methods sample along the feasibility boundary (e.g. EF, PBE, B and R) (Rahat and Wood 2020).

To make PoFV cost-aware, the acquisition value is divided by the predicted cost. Nikova et al. (2023) consider a fixed-cost and cost-cooling strategy for the unknown cost and show their behavior on an engineering problem. Fixed-cost means the influence of the cost stays the same for all iterations, while with cost-cooling the influence of the cost decreases at every iteration. Adding cost-awareness leads to well performing surrogates, while more (feasible) designs are sampled.

Considering σ^2 and $F(\mathbf{x})$ as a two-objective maximization problem, Nikova et al. (2024) create acquisition functions based on *Augmented Tchebysheff (ATCH)* and *Augmented Achievement Scalarizing Function (AASF)* scalarization methods which use a reference point z and weights $\mathbf{w}$ to choose a sample on the Pareto front (Figure 1), while achieving surrogate performance that is better than most state-of-the-art acquisition functions (Figure 2). Depending on the weights in ATCH and AASF, another sample on the Pareto front can be chosen. This results in a greater choice of samples than with other methods. Experiments in Nikova et al. (2024) show that using AASF or ATCH also leads to more feasible designs than the boundary-sampling acquisition functions.

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REFERENCES

De Ath, G., R. M. Everson, A. A. M. Rahat, and J. E. Fieldsend. 2021, apr. "Greed Is Good: Exploration and Exploitation Trade-offs in Bayesian Optimisation". *ACM Trans. Evol. Learn. Optim.* 1(1) https://doi.org/10.1145/3425501.

Nikova, I., I. Couckuyt, and T. Dhaene. 2022. "Data-Efficient Feasible Region Identification for Engineering Design". In *Faculty of Engineering and Architecture Research Symposium 2022 (FEARS 2022), Abstracts*, 1 https://doi.org/10.5281/zenodo.7405492.

Nikova, I., T. Dhaene, and I. Couckuyt. 2023. "Cost-Aware Active Learning for Feasible Region Identification". In *Proceedings of the Companion Conference on Genetic and Evolutionary Computation*, GECCO '23 Companion, 2286–2288. New York, NY, USA: Association for Computing Machinery https://doi.org/10.1145/3583133.3596323.

Nikova, I., S. Rojas Gonzalez, T. Dhaene, and I. Couckuyt. 2024. "Trade-Offs in Bayesian Active Learning for Feasible Region Identification". under review.

Rahat, A. and M. Wood. 2020. "On Bayesian Search for the Feasible Space Under Computationally Expensive Constraints". In *Machine Learning, Optimization, and Data Science*, Volume 12566 of *Lecture Notes in Computer Science*, 529–540. Springer International Publishing https://doi.org/10.1007/978-3-030-64580-9_44.