Quantum Annealing-Driven Active Learning Benchmark for Nanophotonic Design

Serang Jung[1] Jiho Lee[1] Jungmin Gwon[2] Eungkyu Lee[3] Youn Sang Kim[1]

1Department of Chemical and Biological Engineering, College of Engineering, Seoul National University, Seoul, Republic of Korea

[2]Samsung Electronics, Pyeongtaek-si, Republic of Korea

[3]Department of Electronic Engineering, Kyung Hee University, Yongin-si, Republic of Korea

Correspondence to: Youn Sang Kim younskim@snu.ac.kr

1. Introduction

Designing nanophotonic structures requires optimization over high-dimensional parametric spaces, where exhaustive search is computationally infeasible. To tackle this, machine learning—especially active learning—has been widely adopted to efficiently navigate the design space. In active learning, a surrogate model is trained to predict the performance (figure-of-merit, FOM) of candidate designs, and optimal candidates are iteratively selected through an optimization algorithm. Various regression models and optimization techniques can be used in this framework, including conventional algorithms and quantum annealing (QA) [1]. This study aims to benchmark the performance of different combinations of regression and optimization methods within an active learning framework, focusing on comparing QA with classical optimization approaches.

2. Results and Discussion

The active learning framework in this study follows a four-step iterative process: (1) constructing a surrogate model from the training dataset consisting of (binarized design, FOM) pairs using a regression algorithm, (2) identifying the optimal design through optimization, (3) evaluating the FOM of the proposed design, and (4) augmenting the dataset with the new (binarized design, FOM) pair and repeating the cycle [2,3].

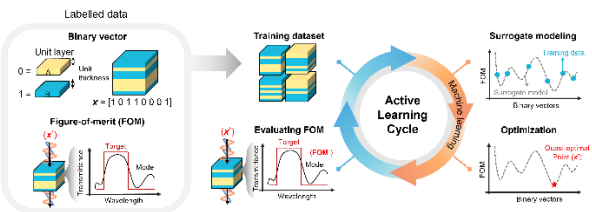

Fig. 1: Active learning process

This framework presents two primary challenges: (i) developing a regression model that accurately captures the FOM landscape over the parametric space, and (ii) efficiently locating the global optimum of the surrogate model. To systematically address both, we conducted a benchmarking study of various regression and optimization combinations. Here, three surrogate models—factorization machine (FM), Gaussian process regression (GPR), and convolutional neural network (CNN)—were evaluated. For optimization, we employed both particle swarm optimization (PSO) and quantum annealing (QA). Binary design tasks ranging from 17 to 50 bits were tested.

Results show that FM, GPR, and CNN achieved comparable R^2 scores, indicating similar regression accuracy across surrogate models. However, in terms of optimization performance, the FM+QA combination consistently discovered designs with lower FOMs, particularly in high-bit scenarios. Additionally, FM+QA demonstrated the shortest runtime per active learning cycle, confirming its computational efficiency. To further evaluate optimization capability independent of surrogate accuracy, we tested QA and PSO using identical quadratic unconstrained binary optimization (QUBO) matrix formulations derived from FM outputs. QA consistently outperformed PSO by finding lower FOMs across all problem sizes, validating its robustness as a global optimizer within the active learning framework. These findings suggest that integrating QA with a lightweight yet expressive model like FM enables efficient and scalable optimization in nanophotonic design tasks.

References

[1] Kim, S. et al., “Quantum annealing for combinatorial optimization: a benchmarking study”, npj Quantum Inf 11, 77 (2025).

[2] S. Kim et al., “Wide-angle spectral filter for energy-saving windows designed by quantum anneling-enhanced active learning, 5, 101847 (2024).

[3] Yu, J. et al., “Ultrathin Ge-YF_3 antireflective coating with 0.5 % reflectivity on high-index substrate for long-wavelength infrared cameras”, Nanophotonics, 13,21, 4067-4078 (2024).