CMSC 35360 Autonomous Laboratories HW1

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Introduction:

Sterling Baird's light-mixing SDL-Demo is a self-driving lab demonstration that showcases the capabilities of autonomous laboratories in the context of a simple experiment involving light mixing. This task provides implementations of grid search, random search, and Bayesian optimization for a color mixing task using one of the Jupyter Notebooks from the project. We ran a remote version of the experiment with 8 different RGB target configurations for a constant seed and recorded notable results below. We also ran the experiment 4 times varying the seed for the experiment with a constant target RGB of R25_G25_B25.

Analysis

After analyzing the data we collected from our eight tests, we observed a variety of trends when comparing the various optimization methods. In our first round of experiments, we held the seed value constant while varying the target RGB values.

In this first experiment, by analyzing the Frechet distance and best estimate graphs, we see a similar trend: Bayesian optimization generally outperforms both random and grid search (figure 2). For instance, in one execution, the median Frechet distance from the points to the target in the RGB space did not exceed 30, while the average distance for both the grid and random search cases did (figure 5). Furthermore, we observed that random search generally produces better final results than grid search (compare the Frechet distances in figure 5. Also, figure 4 exemplifies the smaller final error for random search), with the only exception being when the target was on the grid (figure 3). In this case, grid search outperformed the other two methods, since the target value was one of the RGB values it was searching for through the grid. Additionally, when analyzing the best error attained so far after multiple iterations, we observe a similar trend whereby the Bayesian approach convergest to the best error the fastest, followed by random and then grid search (figure 4).

In our second round of experiments, we held the target RGB values constant while varying the seed number. Within this group of experiments, we saw largely the same trends as those found in the varying RGB experiment (figure 7 shows a similar pattern of Frechet distances), with the Bayesian optimization method consistently producing the best estimate (as exemplified by figure 8). We did see more variation in the starting performance (compare, for example, the starting error for the Bayesian method across figure 6), but over the iterations the trends normalized to what was expected from our previous experiments. More specifically, Bayesian performed the best and consistently normalized to a best error of approximately 500, while the random value approach normalized to a value of nearly 2100, and the grid search plateaued at the closest grid point resulting in a best error rate of approximately 2700 (figure 6).

Results (Constant Seed)

8 RGB Configurations:

R25_G25_B25,R25_G25_B65,R25_G65_B25,R65_G25_B25
R25_G65_B65,R65_G25_B65,R65_G65_B25, R65_G65_B65

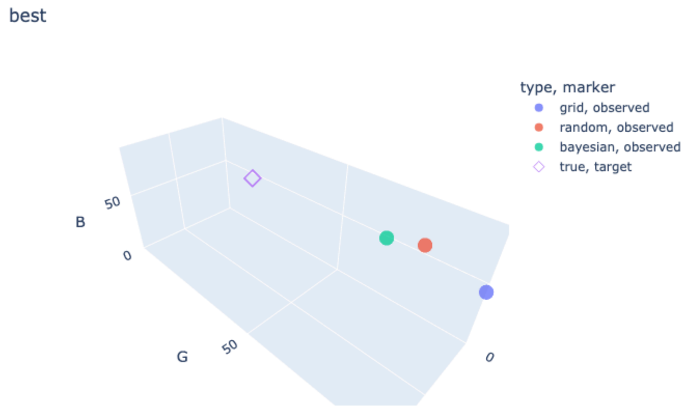

Figure 1: Target: R25_G25_B65: Worst Bayesian Final Model Performance

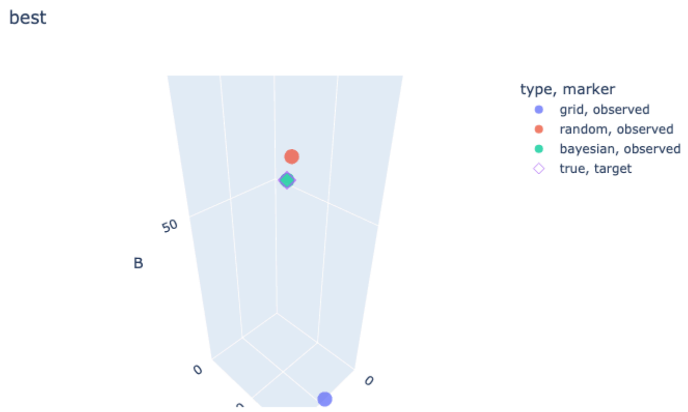

Figure 2: Target: R65_G65_B65: Added Dimensionality Decreases Grid Performance

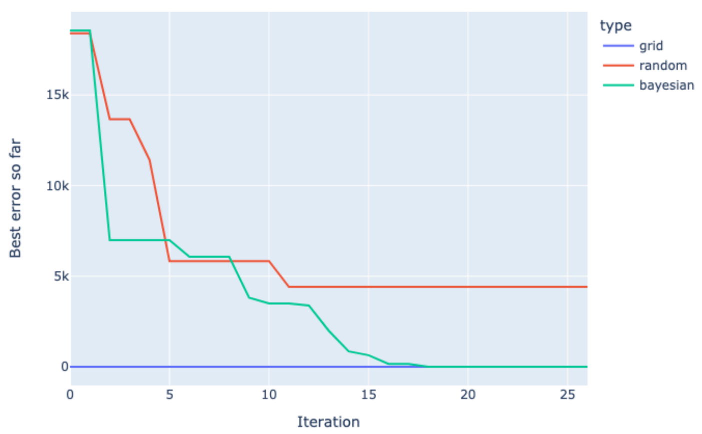

Figure 3: Target: R0_G0_B0: Grid Search Is Optimal for Target on Grid

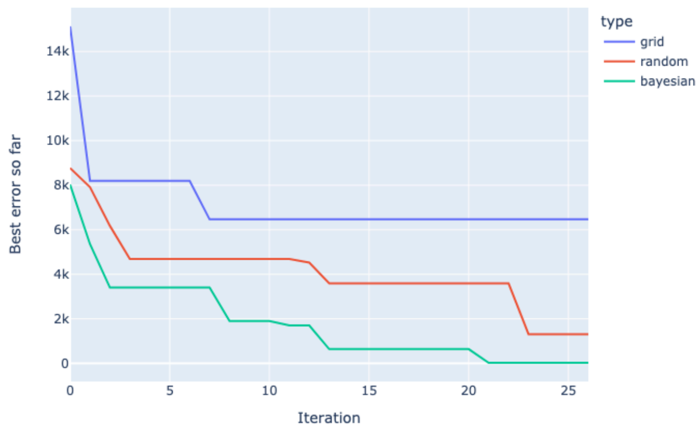

Figure 4: Target: R65_G65_B65: Bayesian and Semi-Random Search Outperform Grid

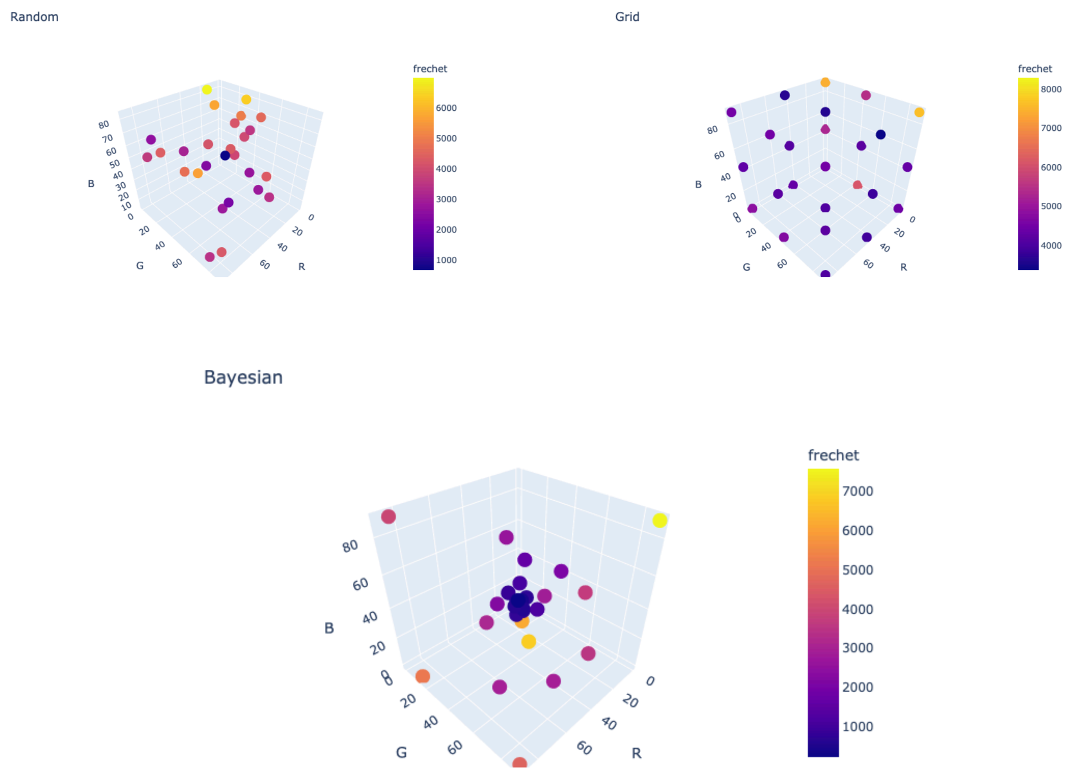

Figure 5: Target R65_G25_B65, Frechet distances for different optimization methods

Results (Random Seed)

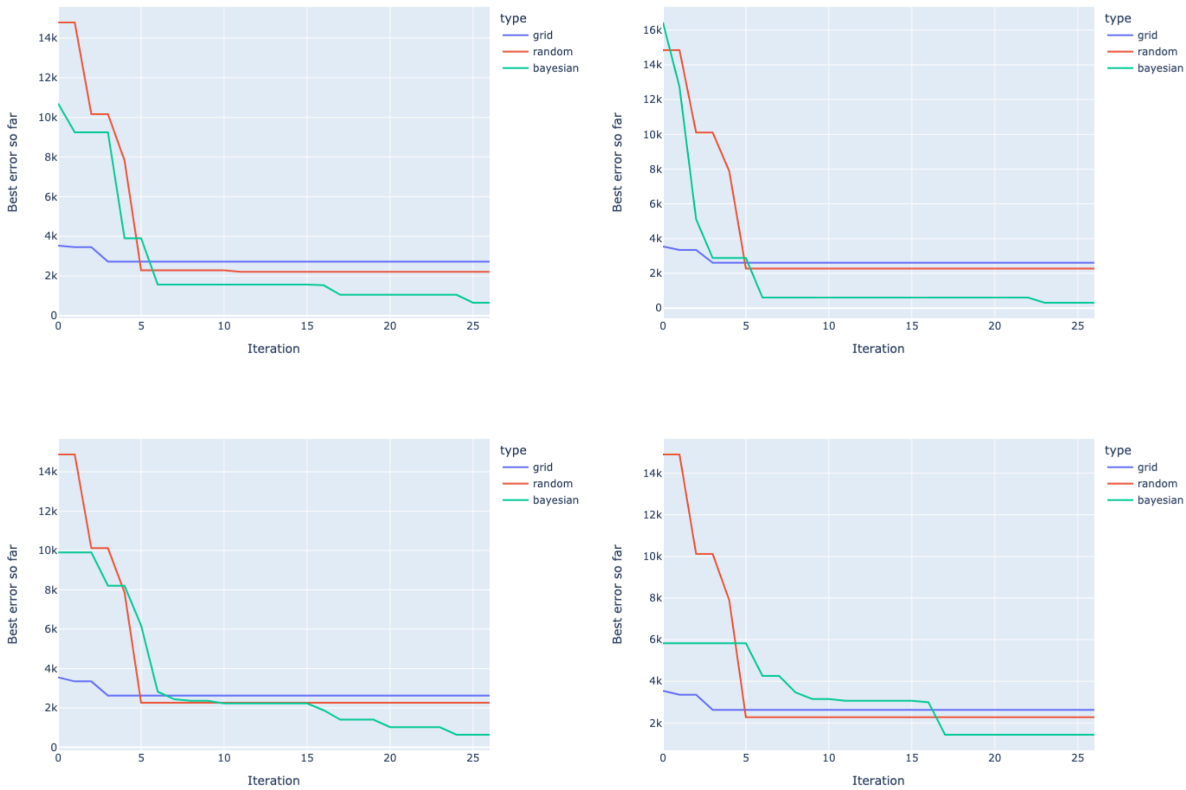

Figure 6: Grid of best error estimate across multiple iterations for each of the four different seeds.

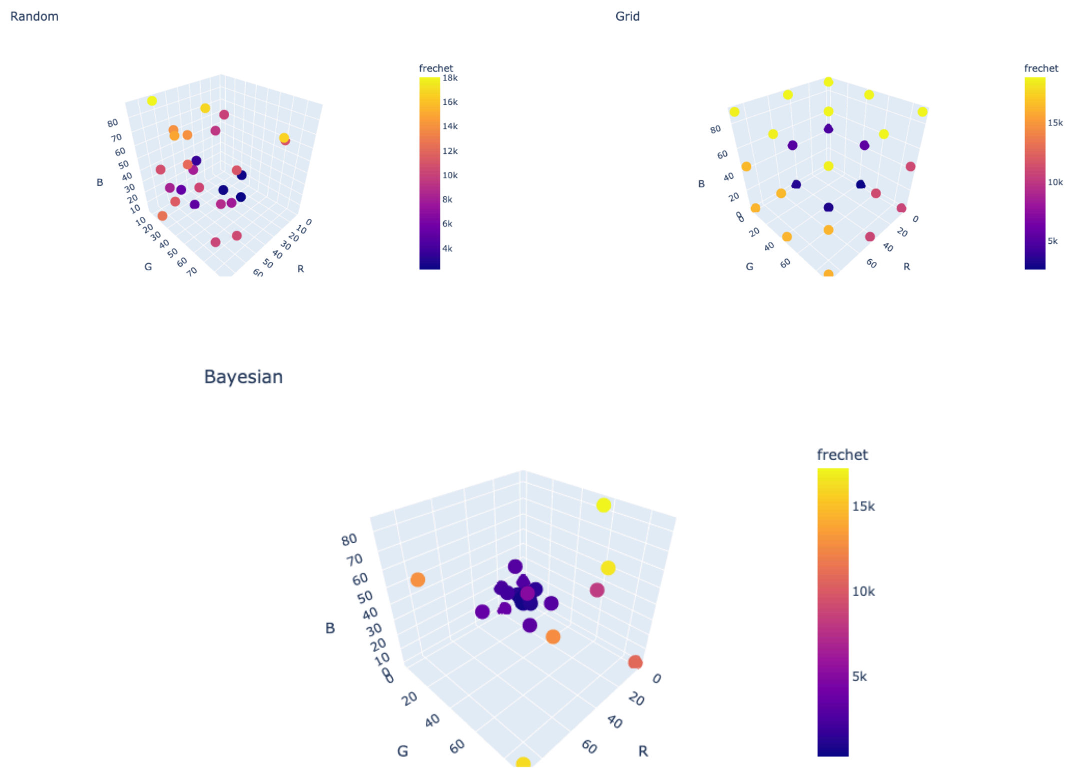

Figure 7: Second random seed, Frechet distances for different optimization methods

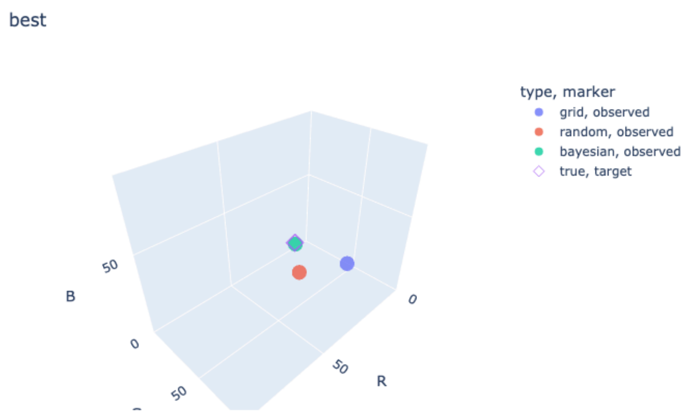

Figure 8: First Random Seed Model Performance