[IE801] SPECIAL TOPICS IN INDUSTRIAL ENGINEERING II - MANUFACTURING & AI

HW #2

Due: 11:59 PM, April 22

Introduction

This assignment focuses on practicing the implementation of algorithms covered in class and finding optimal control settings for the steel industry case study. Part I involves implementing the algorithms, while Part II focuses on applying these algorithms to the case study. You are required to use your implementations from Part I to complete the tasks in Part II.

Homework Tasks

Part I

A. Particle Swarm Optimization (PSO)

- Implement the PSO algorithm as a single function using primitive functions (i.e., without using existing PSO libraries). This function must accept the following input arguments: objective function, maximum iterations (termination occurs after this number of iterations), swarm size, lower and upper bounds, inertia weight, and acceleration coefficients.
- Modify your original PSO implementation to include the auto hyperparameter adjustment capability described on page 15 of the PSO lecture slides.
- Apply both PSO implementations to the optimization problem given on page 10 of the PSO lecture slides and report the optimal solutions.

B. Gaussian Processes (GP)

- Implement the GP algorithm using primitive functions only (no external GP libraries). Specifically, implement three separate functions:
  (1) Squared exponential covariance (kernel) function.
  (2) A function to optimize hyperparameters of the kernel function (you may use a nonlinear optimization library for this purpose).
  (3) A GP prediction function taking as input: the training dataset (input-output pairs), a test set of input points for prediction, and the optimized kernel hyperparameters.
- Validate your GP implementation using the provided dataset (`goldstein_price.csv`). Reproduce the 3D plots shown on page 186 of the GP lecture slides to demonstrate correctness.

Part II

A. Neural Networks + Quasi-Newton Optimization

- Using the provided dataset (`coating_sampled.csv`), train prediction models where the input variables include `thickness`, `width`, `speed`, `tension`, `gap`, `pressure`, and `angle`. Among these, `gap` and `pressure` are treated as control variables, while the rest are environmental variables. The output variable is `weight`. Note that the steel strip has two sides (top and bottom), so you must build separate models for each side. For predictive modeling, use neural networks. You may use existing neural network libraries for training. Report prediction accuracy using evaluation methods and plots of your choice (e.g., predicted vs. actual plot, R-squared, etc.).
- Next, we aim to find optimal control values (gap and pressure) that achieve target weight

values. Consider the scenario of real-time coating weight control discussed in the Case Study I lecture slides. Specifically, use the first 16 instances in the dataset that correspond to coil CRG2188. Assume that gap and pressure values are unknown and that the given weight values are the target values. Your task is to find optimal control values that minimize the difference between predicted and target weights by solving the nonlinear optimization problem described on page 14 of the Case Study I lecture slides. Implement the corresponding objective function, and solve the optimization problem using the quasi-Newton method (BFGS algorithm). You may use existing optimization libraries. Perform this procedure for both the top and bottom sides. Note that the environmental input variables are provided in the dataset for those 16 instances. Verify that your implementation works by checking whether the optimization recovers reasonable gap and pressure values. If discrepancies exist between the predicted and actual gap/pressure values, provide possible explanations.

B. Gaussian Processes + (PSO, Quasi-Newton Optimization)

- Repeat the procedure described in Part II-A using Gaussian Processes for predictive modeling. For the optimization step, apply both PSO and the quasi-Newton method (BFGS algorithm) to find the optimal control values. You must use your own implementations of Gaussian Processes and PSO from Part I.

C. Gradient Boosting + PSO

- Again, repeat the procedure described in Part II-A using Gradient Boosting for predictive modeling and PSO for optimization. You must use your PSO implementation from Part I. For Gradient Boosting, you may use existing libraries.

D. Bayesian Optimization

- In this section, you will apply Bayesian Optimization (BO) to search for optimal control settings under a process change scenario with limited data. Examine the dataset (`coating_sampled.csv`) and identify the transition point where the coil changes from CRG2188 (the first coil) to the next one. Notice that there is a significant shift in control variables such as `gap_top` and `pressure_top` across this boundary.
- Assume this represents an online adaptation scenario where a model trained on the first coil is no longer reliable due to a process shift. Your objective is to find optimal values for the control variables (gap and pressure) to achieve the target coating weight under the new condition (i.e., for the second coil).
- Select a small number of initial observations (e.g., 5–10 instances) from the second coil to use as initial data. Then, using Bayesian Optimization:
  (1) Fit a surrogate model (use your GP implementation from Part I or a GP-based BO library),
  (2) Use an acquisition function such as Expected Improvement (EI) to efficiently explore the control input space,
  (3) Keep the environmental variables (thickness, width, speed, tension, angle) fixed to the values provided in the dataset (More precisely, for each instance at time t, the environmental values are those observed at time $t-1$.), and treat `gap_top` and `pressure_top` as the only control variables to be optimized. (*Hint: Consider an acquisition function conditioned on the environmental variables.*)
  (4) Determine the next control settings for `gap_top` and `pressure_top`.
- For simplicity, focus only on the top side in this task.
- In your report, include:
  (1) A description of how you selected the initial dataset.
  (2) Plots of gap, pressure, and coating weight, including your control settings and the predicted coating weight.

(3) A discussion on the advantages and limitations of Bayesian Optimization in this adaptive control setting, particularly under conditions with limited data and nonstationary behavior.
(4) Feel free to suggest any ideas for using the previously trained prediction model.

Notes

- Submit your code and results by uploading the files to the KLMS system.
- While students may use AI tools for guidance, they must fully understand their implementations.
- After designing all the homework problems, it seems that the total workload may be a bit too much to complete by the due date. Therefore, the Bayesian Optimization (Part II-D) section is optional for the original deadline. If you are able to complete it, please submit it by the regular due date. Otherwise, you may submit Part II-D only by 11:59 PM, April 29. If you wish to submit this part separately, please email it directly to our TA at chanh99kim@kaist.ac.kr.