Fundamentals of Smart Systems Ch En 5205 / 6205

Assignment 8 | Real-Time Optimization (RTO) #2 | Due Tuesday, April 11th at 5 PM

In this assignment, we will try to improve the performance of the plant by using a different RTO methodology. The model we used for optimization in Assignment 7 (which we fit using ML models in Assignment 6) had inaccuracies, which caused plant/model mismatch. This meant that our "optimal" solution was not always the true optimum. We will use a more accurate model of the plant in Assignment 8 to see how performance can be improved by improving model accuracy. Additionally, there were times in Assignment 7 where the plant lost money due to unfavorable economics. In Assignment 8, we are going to explore the idea of idling the reactor when the economics are unfavorable. We won't be able to prevent days with negative profitability, but we will try to mitigate the severity of these losses. Carefully read through the table below to understand how we'll approach optimization differently this time.

Assignment 7 Methodology	**Assignment 8 Methodology**
We used a data-driven model, derived from operating data of the reactor and using ML tools to fit the model.	We will use a first principles or physics-based model, derived from knowledge of the actual governing equations of the reactor.
Our plant model was essentially built into the objective function of the optimization problem.	Our plant model will be built into equality constraints of the optimization problem.
Our model used a quadratic approximation of the plant.	We will use a more complex, nonlinear (but still steady state) model of the plant.
The optimization model was convex, meaning that an optimal solution found was guaranteed to be the global optimum.	This optimization problem is not necessarily convex, meaning that the solver may converge on local optima and may be able to find better solutions if given a different initial guess.
We considered only two degrees of freedom (q and Q_B), assuming all other variables would be constant (like h), dependent on other variables (like Q_A), or an uncontrollable disturbance (like the inlet temperatures and concentrations).	We will now introduce an extra degree of freedom into the optimization. Rather than hold the level (h) constant, we will allow it to fluctuate within a set of bounds.
There were no equality constraints, so the degrees of freedom (DOFs) were just the 2 decision variables.	We will now enforce our model through equality constraints. These will be the 5 balances from Assignment 1. We'll have 8 decision variables and 5 equality constraints, leaving us with 3 DOFs.

1- Reformulate the Jupyter Notebook optimization problem from Assignment 7. This time, use the following 8 decision variables, with the associated lower and upper bounds. These 8 variables will make up your x vector of decision variables as inputs.

Variable	Description	Units	Lower Bound	Upper Bound
C_A	Concentration of A in reactor	kmol/m^3	0	20
C_B	Concentration of B in reactor	kmol/m^3	0	20
C_C	Concentration of C in reactor	kmol/m^3	0	10
T	Reactor Temperature	K	300	620
h	Reactor level (or height)	m	1	8
Q_A	Inlet flow of component A	m^3/min	1	8
Q_B	Inlet flow of component B	m^3/min	1	8
q	Heat input to reactor	GJ/min	0	12

a. Update the objective function. You'll still use negative profit as the objective function, but rewrite the it using the relevant decision variables (you won't need all of them) and the costs, which will still be passed through as arguments. **Show your code containing the objective function and the definition of decision variables.**

b. Update the constraints function. Use the original balance equations from your Collimator model (the volume balance, the component balances, and the energy balance) to formulate equality constraints representing the reactor physics. Optimization will be based on steady-state operation, so the optimization problem needs to be set up so that the left-hand side of all of these equations can be solved for zero. Because it is steady-state optimization, you can also zero out / delete any derivative terms (dX/dt) on the right-hand side. You can also multiply both sides of the equation by volume to eliminate it in the denominator. You can define constants or intermediate variables before / in the middle of the key equality constraint equations. Use 400 K for the inlet temperatures and 15 kmol/m^3 for the inlet concentrations. **Show your code containing the constraints function.**

c. Update your initial guess and the bounds in your code to accommodate the 8 decision variables listed in the table above. Choose an initial guess for each variable that is within the bounds. Ensure that the main line of code using the minimize command has all of the inputs it needs. **Show your code containing the updated bounds, initial guess, and minimize command.**

2- Solve the optimization problem with the costs shown in the table below. The solution should give you the optimal value of all eight decision variables. Inspect these after each solve to ensure that they make physical sense and that all constraints are being satisfied. Since there are only three degrees of freedom, we'll take a closer look at only three of the decision variables, which will eventually be pushed down to our plant (Collimator model) for RTO.

   a. **Complete the table by filling in the optimal values and the profitability in each scenario.**

$Cost_A$ (\$/m^3)	**$Cost_B$ (\$/m^3)**	**$Cost_C$ (\$/kmol)**	**$Cost_q$ (\$/GJ)**	**Q_B* (m^3/min)**	**q* (GJ/min)**	**h* (m)**	**Profit (\$/min)**
2	5	5	2				
2	50	20	2				
2	10	5	20				
20	50	2	20				

   b. **In the last scenario, please explain what the optimizer is trying to do?**

3- With the optimization problem formulated and solving, implement a real-time optimization (RTO) application where the optimization solver takes in the commodity prices for the day, solves for optimal Q_B, q, and h based on those prices, and implements these optimal decisions in the "plant" (i.e., the Collimator Simulation). You will need to use some of the API commands you used in Assignment 7 to push optimal set points to the plant and gather the results. Solve this for the whole year using the same prices and random number seeds as in Assignment 7. Be sure to save your results to a CSV file with a new name and/or in a new folder so you don't overwrite the results from Assignment 7.

   a. **What is the total profit for the year when you optimize daily based on commodity prices using this methodology?**
   b. **What is the percent increase in profit compared to not optimizing?**
   c. **What is the percent increase in profit compared to the optimization method used in Assignment 7?**
   d. **Plot profit vs. time for each day in three scenarios: First Principles Optimization (Assignment 8), ML Optimization (Assignment 7), and No Optimization (Assignment 7). You can do this in PowerBI (preferred), Python, or Excel. Show this plot. You can show a zoomed in version (e.g., for ~one month) to better show the differences.**
   e. **Plot total profit vs. time for each day in all three scenarios scenarios in PowerBI (preferred), Python, or Excel. Show this plot.**
   f. **If your results show that profitability increased using this updated methodology, can you give some reasons why?**