PROJECT

Project Report Submitted in partial fulfilment of the requirements

of the Course

CH-5150: Optimization Techniques I

By

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M. Tech. in Climate Change

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Declaration

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Place: IIT HYDERABAD

Problem

For the autocatalytic reaction happening in an isothermal batch reactor as described below, find optimal k1 and k2 values. Using the optimal k1 and k2 values, find the time at which CB maximizes and the corresponding maximum value of CB. Do not find the maximum value of CB and the time at which it occurs, directly from the solution of the ode solver. For both questions, solve the ODEs using an ode solver and, find the optimal k values, time with a suitable minimization solver, and report the observations. (Use the data given in Autocatalytic_Rxn_1.xlsx to solve for k1 and k2. In the Autocatalytic_Rxn_1.xlsx, 1st column is time span, and 2 to 4 columns are CA, CB, and CC).

Rate equations:

$$\frac{dC_A}{dt} = -k_1 C_A C_B$$

$$\frac{dC_B}{dt} = k_1 C_B C_A - k_2 C_B$$

$$\frac{dC_C}{dt} = k_2 C_B$$

METHODOLOGY

- We first load the data from the excel sheet. The concentration data was obtained from an Excel file (Autocatalytic_Rxn_1.xlsx), which includes time and concentration values for A, B, and C.
- **Defining Rate equations:**
    - dCA/dt = - (k1*CA*CB)
    - dCB/dt = (k1*CA*CB) - (k2*CB)
    - dCC/dt = (k2*CA)

1. The above rate equations are utilized to describe how the concentrations vary with respect to time.
2. These equations give the rate of change of each species. They are called as rate constants i.e., k1 and k2.

- ## Optimization Models used:

I have used different optimization algorithms and methods provided in the SciPy library to find the optimal values of k1 and k2. Four optimization methods were implemented using the 'scipy.optimize.minimize' function are:

a. SLSQP (Sequential Least SQuares Programming)
b. Powell
c. Nelder Mead
d. L-BFGS-B (Limited Memory-BFG- Bounded Constraints)

- ## Define the objective function which is subjected to optimization:

I have defined the objective functions in such a manner to find that takes rate constants (k1 and k2) as constants, and then solves the ODE using the constants, and then minimizes the sum of squared errors between the data and model parameters. The function is defined as:

$$\textbf{Objective} = \sum((CA,model - CA)^2 + (CB,model - CB)^2 + (CC,model - CC)^2)$$

- ## Optimization process:

The optimization process minimizes this error by adjusting the rate constants. For each method, the optimization algorithm repeatedly refines the rate constants to minimize the error.

- ## Initial Guess:

I provide an initial guess for the rate constants (k1 and k2). The initial values act as starting points for the optimization process. Here I have set the initial guess to [0.1, 0.1]. I used this as it is a common method in optimization solving.

- ## Results:

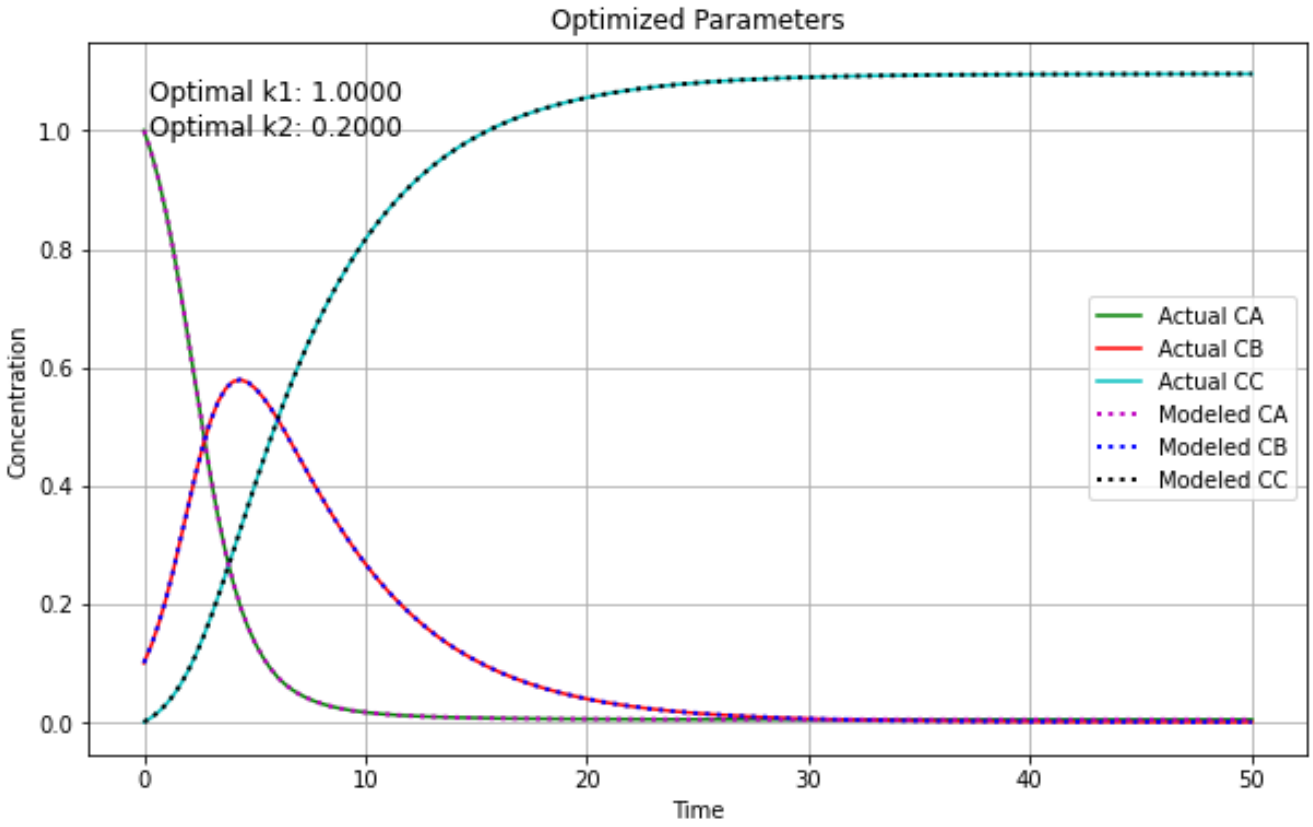
After we have executed each optimization method, we store the optimized rate constants and the errors. From this we also can compare the performance of all the methods to determine which one provides the best fit to the given data by the following error calculation method:

1. **Root Mean Squared Error Calculation for Each Species:** The function calculates RMSE for CA, CB, and CC separately, giving insight into how well the model predicts each concentration.
2. **Overall Root Mean Squared Error:** The overall RMSE is then computed by averaging the individual RMSE values. This provides a single metric that reflects the model's performance across all species.

The optimized parameters and outputs for each method is as given below:

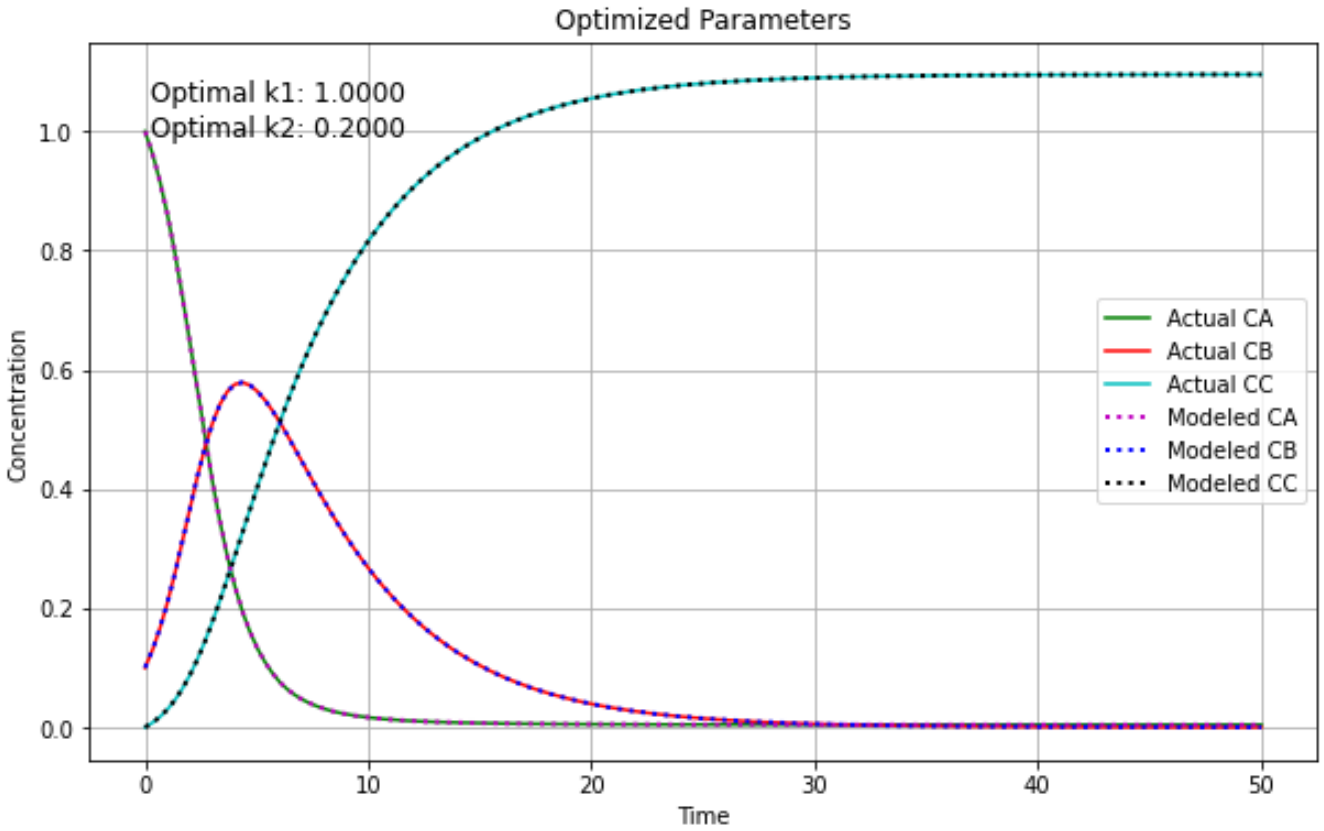
1. SLSQP

- k1: 0.9999728859531203
- k2: 0.19995510068367003
- Time at which CB maximizes: 4.36241610738255
- Maximum value of CB: 0.5787649143918681
- Root Mean Squared Error: 2.5652857888026098e-05



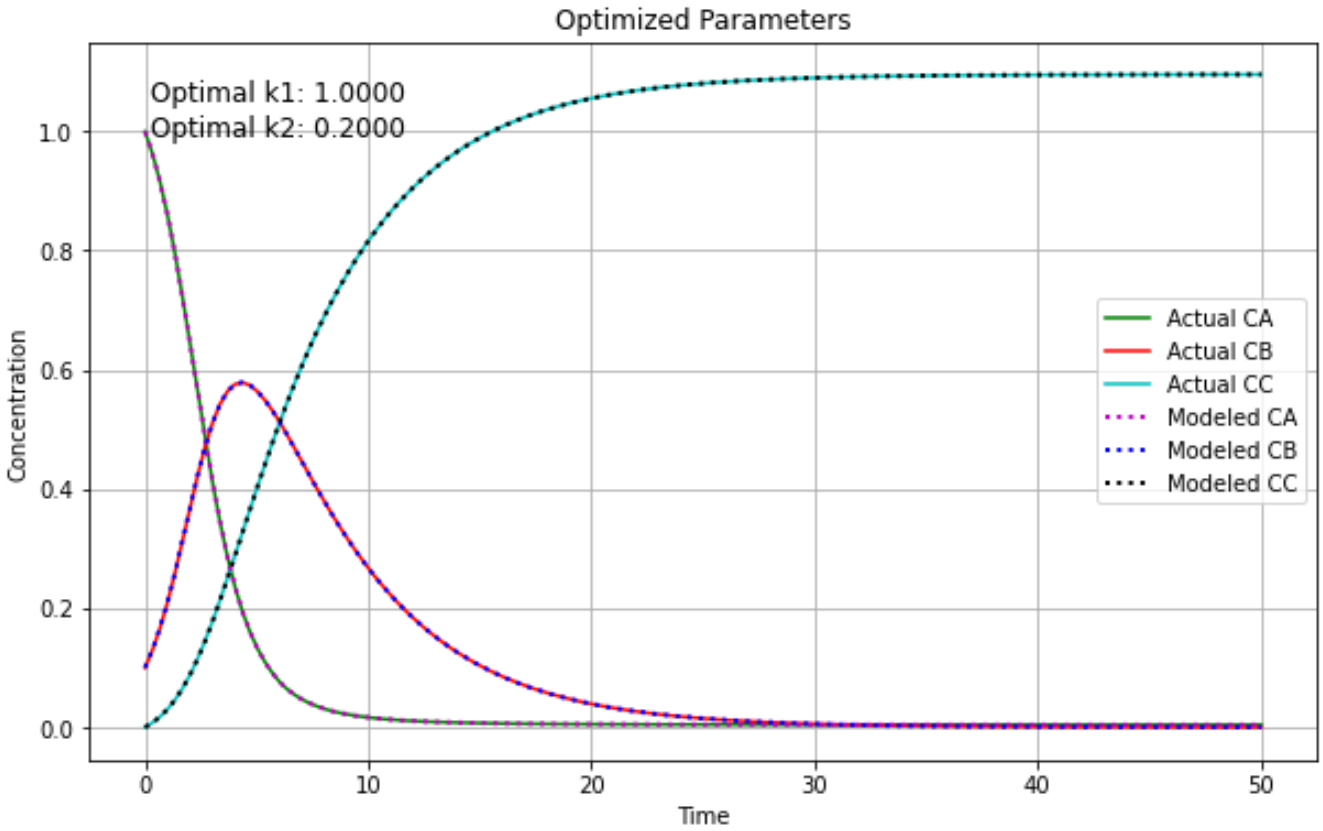
2. Powell Method

- k1: 1.0000011792659607
- k2: 0.20000012116413932
- Time at which CB maximizes: 4.36241610738255
- Maximum value of CB: 0.5787009656795716
- Root Mean Squared Error: 2.1164996051938388e-07



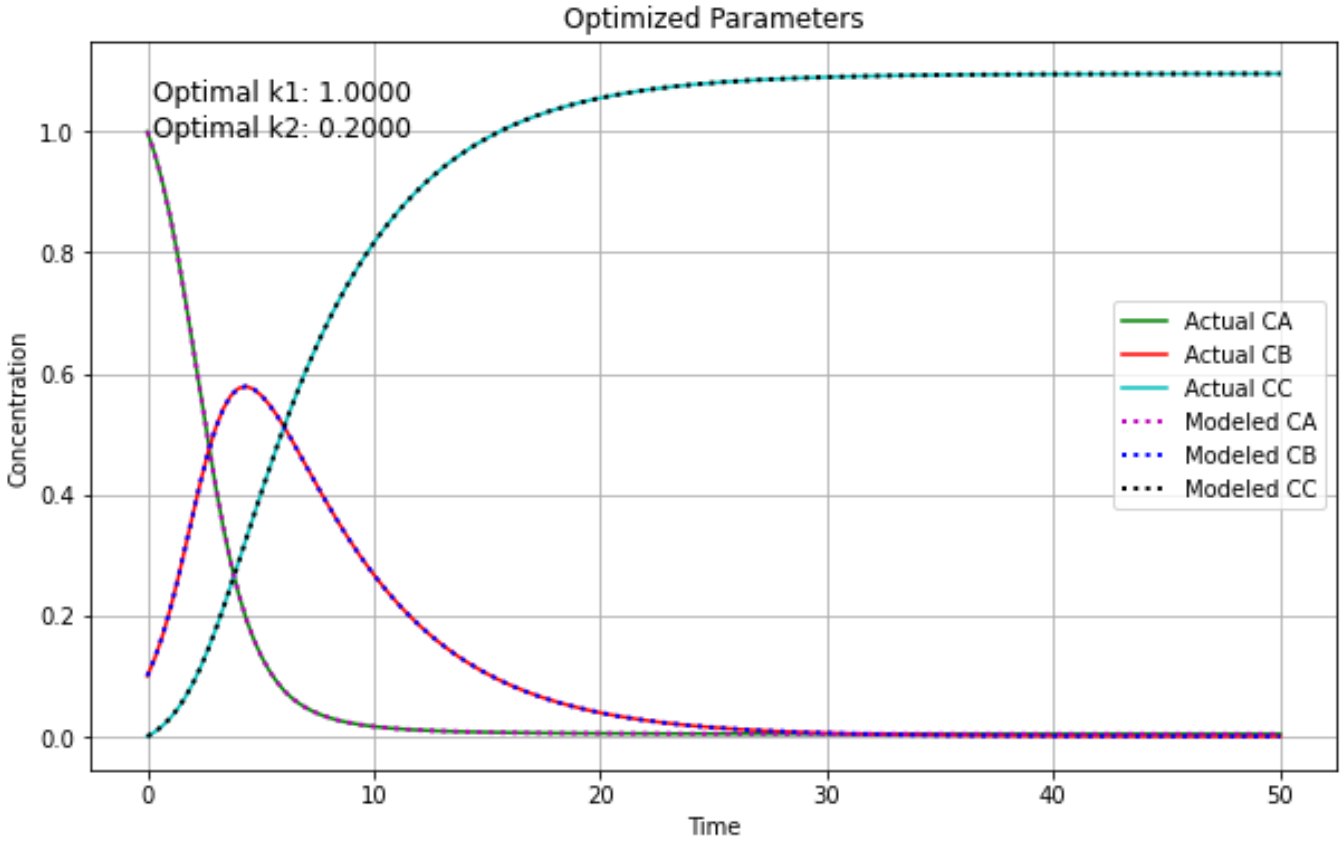
3. Nelder-Mead Method

- k1: 0.9999614263447297
- k2: 0.19999779055249822
- Time at which CB maximizes: 4.36241610738255
- Maximum value of CB: 0.5786924898487843
- Root Mean Squared Error: 6.4336031869830275e-06



4. L-BFGS-B Method

- k1: 0.9999997963474021
- k2: 0.19999998848858977
- Time at which CB maximizes: 4.36241610738255
- Maximum value of CB: 0.5787007541298023
- Root Mean Squared Error: 3.392758362892257e-08



- ## Conclusion

- The best optimization method was determined to be the **L-BFGS-B** optimization algorithm which yielded the most accurate results, as evidenced by the **lowest Root Mean Squared Error (RMSE) value of 3.392758362892257e-08 across all three species** and the following parameters:
  i. k1: 0.9999997963474021
  ii. k2: 0.19999998848858977
  iii. Time at which CB maximizes: 4.36241610738255
  iv. Maximum value of CB: 0.5787007541298023

- This comprehensive evaluation of the model's fit demonstrated that the optimized parameters effectively describe the concentration dynamics of the reaction over time.