

CHBE 552 Problem Set 1

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Question 1

By implementing SA method with following parameters: bounds = $(-1, 1)$, initial temperature = 10000, cooling rate = 0.95, stopping temperature = 0.001, and max iterations = 1000, three tests are conducted and the results are shown as following:

Test 1:

Best x_1 and x_2 are $[0.00016685, -0.00014399]$ and the best function value is $1.074285020 \cdot 10^{-6}$.

Test 2:

Best x_1 and x_2 are $[0.00019128, 0.00056343]$ and the best function value is $1.08674897771 \cdot 10^{-5}$.

Test 3:

Best x_1 and x_2 are $[0.00023714, 0.00051509]$ and the best function value is $9.45038628186 \cdot 10^{-6}$.

Thus, one can conclude the best x_1 and x_2 are $[0, 0]$ and the best function value is 0. The tiny error might comes from the numerical uncertainty of float computation in Python.

Question 2

By implementing Luus-Jaakola method according to the reference with such parameters:

Initial guess of each x_j : $x_{bounds} = [(0, 1)]$

max iterations: $N = 10000$

Initial search area: $V_{initial} = 0.1$

Search area reduction factor: $V_r = 0.999$

Solution for variables x_1 to x_{10} are found to be

$$\begin{aligned}x_1 &= 0.0406700206 \\x_2 &= 0.147744627 \\x_3 &= 0.783102950 \\x_4 &= 0.00141387372 \\x_5 &= 0.485248112 \\x_6 &= 0.000691530012 \\x_7 &= 0.0273983722 \\x_8 &= 0.0179474168 \\x_9 &= 0.0373039831 \\x_{10} &= 0.0969432948\end{aligned}$$

And the optimal objective function value is computed to be -47.7610, which generally agrees with the value provided in the reference paper.

Note that the number of iterations are set to be very high such that a global minimum could be found, and the search area reduction factor is close to 1 such that the search area only reduces a little bit in each iteration, thus, the solution of x_j could have more digits.

Question 3

By implementing Luus-Jaakola method according to the reference with same parameters stated in question 2, except for initial guess of x_j since the bounds should follow the indicated constraint in the paper:

Best Solution for independent variable:

$$\begin{aligned}x_1 &= 1727.77228 \\x_7 &= 94.25960 \\x_8 &= 10.41761\end{aligned}$$

Dependent Variables:

$$\begin{aligned}x_2 &= 0.000160000000 \\x_3 &= 0.994398201 \\x_4 &= 0.00305494307 \\x_5 &= 0.00199925826 \\x_6 &= 0.908309867 \\x_9 &= 2.56910919 \\x_{10} &= 0.0149778787\end{aligned}$$

Best Objective Function Value: 1161.45677

The results generally agree with the value provided in the reference paper.

Question 4&5

By implementing Nelder-Mead algorithm in Python, for function in part 1: the minimum point is $[0.99999871 \approx 1, 0.99999707 \approx 1]$, and the minimum function value is $1.3556651538450528e-11 \approx 0$.

For function in part 2: the minimum point is $[6.50737582e-04 \approx 0, -6.52767435e-05 \approx 0, -6.74455549e-04 \approx 0, -6.76241743e-04 \approx 0]$, and the minimum function value is $5.379451007433241e-11 \approx 0$.

Again, The tiny error might comes from the numerical uncertainty of float computation in Python.

Question 6

The work done by the first compressor $C - 1$ is given by:

$$W_{C-1} = \frac{RT_1}{\gamma} \left(\left(\frac{P_2}{P_1} \right)^\gamma - 1 \right) \quad (1)$$

The work done by the second compressor $C - 2$, compressing from P_2 to P_4 , is (since $P_2 = P_3$):

$$W_{C-2} = \frac{RT_1}{\gamma} \left(\left(\frac{P_4}{P_2} \right)^\gamma - 1 \right) \quad (2)$$

The total work W_{tot} is the sum of the work done by both compressors:

$$W_{tot} = W_{C-1} + W_{C-2} \quad (3)$$

$$W_{tot} = \frac{RT_1}{\gamma} \left(\left(\frac{P_2}{P_1} \right)^\gamma - 1 \right) + \frac{RT_1}{\gamma} \left(\left(\frac{P_4}{P_2} \right)^\gamma - 1 \right) \quad (4)$$

Differentiate W_{tot} with respect to P_2 to find the minimum:

$$\frac{dW_{tot}}{dP_2} = \frac{RT_1\gamma}{\gamma} \left(\frac{P_2}{P_1} \right)^{\gamma-1} \frac{1}{P_1} - \frac{RT_1\gamma}{\gamma} \left(\frac{P_4}{P_2} \right)^\gamma \frac{1}{P_2^2} \quad (5)$$

Set the derivative equal to zero and solve for P_2 :

$$0 = \frac{RT_1\gamma}{\gamma} \left[\left(\frac{P_2}{P_1} \right)^{\gamma-1} \frac{1}{P_1} - \left(\frac{P_4}{P_2} \right)^\gamma \frac{1}{P_2^2} \right] \quad (6)$$

Simplify and solve for P_2 :

$$\begin{aligned}0 &= P_2^{\gamma-1} \frac{1}{P_1^\gamma} - P_4^\gamma \frac{1}{P_2^{\gamma+1}} \\ P_4^\gamma &= P_2^{2\gamma} \frac{1}{P_1^\gamma} \\ P_2^{2\gamma} &= P_1^\gamma P_4^\gamma \\ P_2^2 &= P_1 P_4\end{aligned}$$

Take the square root of both sides to find P_2 :

$$P_2 = \sqrt{P_1 P_4} \tag{7}$$

This result indicates that the optimal intermediate pressure P_2 is the geometric mean of the inlet pressure P_1 and the final pressure P_4 .