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 accoording to the reference with such parameters:

$$\begin{aligned} \text{Initial guess of each } x_j\text{:}x_{bounds} &= [(0, 1)] \\ \text{max iterations:}N &= 10000 \\ \text{Initial search area:}V_{initial} &= 0.1 \\ \text{Search area reduction factor:}V_r &= 0.999 \end{aligned}$$

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 setted to be very such that a global minimum could be found, and the search area reduction fractor are 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 accoording 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:

$$
\begin{aligned}
\text{Best Solution for independent variable:} & \\
x_1 &= 1727.77228 \\
x_7 &= 94.25960 \\
x_8 &= 10.41761 \\
\text{Dependent Variables:} & \\
x_2 &= 0.000160000000 \\
x_3 &= 0.994398201 \\
x_4 &= 0.00305494307 \\
x_5 &= 0.00199925826 \\
x_6 &= 0.908309867 \\
x_9 &= 2.56910919 \\
x_{10} &= 0.0149778787 \\
\text{Best Objective Function Value:}1161.45677 &
\end{aligned}
$$

The results generally agrees 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.