1. Debugging Outputs

Question 1

(a) length of schedule: 5940 for 30K, 5980 for 10K. The function evaluation of your solution usually falls in the range of 3000-5000

Question 2

- "pairs" refers to the pairing instruction in 1b, which you need to do every time the population changes
- You can use the following to debug your cross-over and mutate operators

```
In [85]: import numpy as np

def plot_surface(func,x_min=-2,x_max=2,y_min=-2,y_max=2):
    x = np.linspace(x_min,x_max,100)
    y = np.linspace(y_min,y_max,100)
    X,Y = np.meshgrid(x,y)
    Z = func([X,Y])

fig = plt.figure(figsize=(6,3))
    ax = fig.add_subplot(111, projection='3d')
    ax.plot_surface(X,Y,Z, alpha=0.9)
    ax.set_xlabel('x')
    ax.set_ylabel('y')
    # ax.view_init(60,60) # set angles for viewing
    plt.tight_layout()
    plt.show()
```

Simulated annealing code Q1

1a)

```
In [50]: def schwefel(x vector):
             return 418.9892 * len(x_vector) - np.sum(x_vector * np.sin(np.sqrt(np.at
         solution = np.random.uniform(-500, 500, 10)
         # evaluation = schwefel function
         delta = 0.5
         boundary = [-500, 500]
         TSA = 3000
         alpha = 0.5
         low temp 30 = 30
         low temp 10 = 10
         len_{cool_30} = (TSA - low_temp_30) / alpha
         len cool 10 = (TSA - low temp 10) / alpha
         cooling_schedule_30 = np.linspace(start=TSA, stop=low_temp_30, num=int(len_c
         print(f"The length of the cooling schedule for 30K is : {len cool 30}")
         print(f"The length of the cooling schedule for 10K is : {len cool 10}")
        The length of the cooling schedule for 30K is: 5940.0
        The length of the cooling schedule for 10K is: 5980.0
In [47]: result = SA(solution, schwefel, delta, boundary, cooling schedule 30)
         print(result['evaluation'])
        4590.757346257131
In [49]: result = SA(solution, schwefel, delta, boundary, cooling_schedule_30)
         print(result['evaluation'])
        4431,18570896581
In [51]: result = SA(solution, schwefel, delta, boundary, cooling schedule 30)
         print(result['evaluation'])
        4967.847171138068
         The three results for the cooling schedule to 30K are shown above. The three results for
         the cooling schedule to 10K are shown below
```

In [64]: solution = np.random.uniform(-500, 500, 10)

The results do look better when cooling to the lower temperature, as the global minima evaluation decreases (closer to the global minimum)

1b)

```
In [79]: TSA 3k = 3000
         TSA_6k = 6000
         sigma = 1000
         k = 6000
         def create logspace cooling(TSA):
             \# [TSA / (1 + TSA * np.log(1 + i)/(3*sigma)] for i in range(1, k+1)]
             return np.array([TSA / (1 + TSA * np.log(1 + i)/(3*sigma)) for i in rar
         cooling 3k = create logspace cooling(TSA 3k)
         cooling 6k = create logspace cooling(TSA 6k)
         print(f"The length of the log cooling schedule for 3000K is : {len(cooling 3
         print(f"The length of the log cooling schedule for 6000K is : \{len(cooling \in A)\}
         solution = np.random.uniform(-500, 500, 10)
         result = SA(solution, schwefel, delta, boundary, cooling 3k)
         print(result['evaluation'])
        The length of the log cooling schedule for 3000K is: 6000
        The length of the log cooling schedule for 6000K is: 6000
        3530, 1512465460246
In [74]: solution = np.random.uniform(-500, 500, 10)
         result = SA(solution, schwefel, delta, boundary, cooling 3k)
         print(result['evaluation'])
        4199.608272639098
In [75]: solution = np.random.uniform(-500, 500, 10)
         result = SA(solution, schwefel, delta, boundary, cooling 3k)
         print(result['evaluation'])
```

3450.8069313035544

```
In [76]: solution = np.random.uniform(-500, 500, 10)
    result = SA(solution, schwefel, delta, boundary, cooling_6k)
    print(result['evaluation'])

4349.086270974157

In [77]: solution = np.random.uniform(-500, 500, 10)
    result = SA(solution, schwefel, delta, boundary, cooling_6k)
    print(result['evaluation'])

3589.046116217409

In [78]: solution = np.random.uniform(-500, 500, 10)
    result = SA(solution, schwefel, delta, boundary, cooling_6k)
    print(result['evaluation'])

2968.863431869962

For both 3k and 6k, the cooling schedules converge better than linear cooling as they
```

For both 3k and 6k, the cooling schedules converge better than linear cooling as they find a lower global minimum on average

1c)

```
In [95]: geometric_cooling_3k = np.array([(alpha ** n) * 3000 for n in range(0, 10)])
         geometric_cooling_3k
                                            750.
Out[95]: array([3000.
                            . 1500.
                                                          375.
                                                                       187.5
                                                                         5.8593751)
                   93.75
                                46.875
                                             23.4375
                                                           11.71875 ,
In [97]: solution = np.random.uniform(-500, 500, 10)
         result = SA(solution, schwefel, delta, boundary, geometric_cooling_3k)
         print(result['evaluation'])
        4437.716582098562
         solution = np.random.uniform(-500, 500, 10)
         result = SA(solution, schwefel, delta, boundary, geometric_cooling_3k)
         print(result['evaluation'])
        5181,237499138457
In [99]: solution = np.random.uniform(-500, 500, 10)
         result = SA(solution, schwefel, delta, boundary, geometric_cooling_3k)
         print(result['evaluation'])
        4698,450759403982
```

I implemented a Geometric annealing schedule, and it appears that this annealing schedule did not lead to increased convergence (the evaluations of the function on average were higher than when I used logarithmic or linear cooling schedules).

```
In [88]: from scipy.optimize import minimize
```

```
def save step(*args):
    for arg in args:
        if type(arg) is np.ndarray:
            steps.append(arg)
def minimize function(x0, func, method):
    Minimize a function
    Parameters
    x0: np.ndarray
        Starting point
    func: function
        Scalar function to minimize
    method: str
        Method for minimization
    Returns
    res: OptimzizeResult
        Result object of scipy optimization
    res = minimize(
        func.
        x0,
        method=method,
        options={"qtol": 1e-5, "disp":True},
        callback=save_step,
    return res
```

Performing a Conjugate Gradient local optimization technique on my solution using a geometric cooling schedule

After performing local optimization (conjugate gradient), an even better solution was found with a function evaluation closer to 0. The function evaluation converged more closely, dropping from 4698.450759403982 to 2468.209950, so it improved!

2 a)

Encoding A

```
Solution 3 - Vector [1000]

Solution 4 - Vector [0010]

Solution 5 - Vector [0001]

Schema: [*0**] Order = 1, Length: 2-2 = 0
```

Encoding B

```
Solution 3 - Vector [1101]

Solution 4 - Vector [1011]

Solution 5 - Vector [1111]

Schema: [1**1] Order = 2, Length: 4 -1 = 3
```

We will choose Encoding A because for genetic algorithms, we want schema with low order and low length. This is because operations like crossing-over will often disrupt schema with high orders or length, preventing those positive traits from being retained. Instead we want low order and low length schema to decrease the chance of those positive encodings to be disrupted by crossing over

```
In [276... | def one_point_crossover(vec1, vec2, point):
             new_vec1 = vec1[:point] + vec2[point:]
             new_vec2 = vec2[:point] + vec1[point:]
             return new_vec1, new_vec2
         def mutate(vec, point):
             binaryAtPoint = vec[point]
             if binaryAtPoint == 0:
                  return vec[:point] + '1' + vec[point + 1:]
             else:
                  return vec[:point] + '0' + vec[point + 1:]
         def two_point_crossover(vec1, vec2, point1, point2):
             new vec1 = vec1[:point1] + vec2[point1:point2] + vec1[point2:]
             new_vec2 = vec2[:point1] + vec1[point1:point2] + vec2[point2:]
             return new_vec1, new_vec2
         def test_one_point_crossover():
             c1, c2 = one point crossover("0000", "1111", 1)
             if {c1, c2} == {"1000", "0111"}:
                 print("Well done!")
```

```
else:
         raise Exception("Wrong implementation")
 def test_mutate():
     if "0000" == mutate("0100", 1):
         print("Well done")
     else:
         raise Exception("Wrong implementation")
 def test_two_point_crossover():
     c1, c2 = two_point_crossover("0000", "1111",1,3)
     if {c1, c2} == {"0110", "1001"}:
         print("Well done")
     else:
         raise Exception("Wrong implementation")
 test one point crossover()
 test mutate()
 test_two_point_crossover()
Well done!
Well done
```

Well done

Population evaluation code Q2

```
In [270... # Complete the following code to get the below output
          def fitness(x):
              return -(x**2) + 8 * x + 15
          def evaluate population(pop):
              # sort polpulation by their fitness
              pop copy = pop copy()
              pop copy.sort(key = fitness,reverse=True)
              print("Solutions
                                 Vector
                                                Fitness")
              for sol in pop_copy:
                  print("%-13d%-13s%-6d"%(sol,vector_dict[sol],fitness(sol)))
              print("="*20)
              print("Total fitness:", sum([fitness(sol) for sol in pop_copy]))
              print(f'Best solution: {pop_copy[0]} with fitness {fitness(pop_copy[0])}
          # decoding based on encoding A: vector -> solution
          solution dict = {
              "1011": 0, "0011": 1, "1001": 2, "1000": 3, "0010": 4, "0001": 5, "0000": 6, "1010": 7,
              "0100": 8, "1100": 9, "0101":10, "0110":11,
              "0111":12, "1101":13, "1110":14, "1111":15,
          # encoding A: solution -> vector
          vector_dict = dict(zip(solution_dict.values(),solution_dict.keys()))
```

```
# initial population
          pop = [4,7,13,10]
          evaluate_population(pop)
         Solutions
                        Vector
                                     Fitness
         4
                        0010
                                      31
         7
                        1010
                                      22
         10
                        0101
                                      -5
                                      -50
         13
                        1101
         Total fitness: -2
         Best solution: 4 with fitness 31
In [271... # you should get this
          2 b)
In [272... pop = [10, 1, 15, 6, 0, 9]
          pop.sort(key=fitness)
          pop
Out[272... [15, 10, 9, 0, 1, 6]
In [273... evaluate_population(pop)
         Solutions
                        Vector
                                     Fitness
                        0000
                                      27
         6
         1
                        0011
                                      22
                        1011
                                      15
         0
         9
                        1100
                                      6
         10
                        0101
                                      -5
         15
                        1111
                                      -90
         Total fitness: -25
         Best solution: 6 with fitness 27
            1. x = 10, Vector: [0101], Fitness: -5
            2. x = 1, Vector: [0011], Fitness: 22
            3. x = 15, Vector: [1111], Fitness: -90
            4. x = 6, Vector: [0000], Fitness: 27
            5. x = 0, Vector: [1011], Fitness: 15
            6. x = 9, Vector: [1100], Fitness: 6
          Pair 1: x = 15 and x = 6
          Pair 2: x = 10 and x = 1
          Pair 3: x = 0 and x = 9
In [274... def generate pairs(population):
               #Takes a sorted list and returns pairings of least-best fit solutions
```

```
file:///Users/chu/Documents/Class/MSSE_Spring2024/Chem277B/HW%232_MSSE_Cameron_Hu.html
```

pairings = []

```
for i in range(int(len(population)/2)):
    low = population[i]
    high = population[len(population) - i - 1]
    pair = (low, high)
    pairings.append(pair)
    return pairings

b_pairs = generate_pairs(pop)
    print(b_pairs)

[(15, 6), (10, 1), (9, 0)]
```

2 c)

```
In [277... | pair1_1_vector, pair1_2_vector = one_point_crossover("0000", "1111", 1)
         new sol 1 = solution dict[pair1 1]
         new_sol_2 = solution_dict[pair1_2]
         pair1 = [new sol 1, new sol 2]
         pair1_vectors = [pair1_1_vector, pair1_2_vector]
         print(pair1)
         print(f"Solution x=6 is now {new sol 1} with fitness {fitness(new sol 1)}")
         print(f"Solution x=15 is now {new_sol_2} with fitness {fitness(new_sol_2)}")
        [12, 3]
        Solution x=6 is now 12 with fitness -33
        Solution x=15 is now 3 with fitness 30
In [278... pair2_1, pair2_2 = one_point_crossover("0011", "0101", 1)
         new_sol_1 = solution_dict[pair2_1]
         new_sol_2 = solution_dict[pair2_2]
         pair2 = [new sol 1, new sol 2]
         pair2_vectors = [pair2_1, pair2_2]
         print(pair2)
         print(f"Solution x=1 is now {new_sol_1} with fitness {fitness(new_sol_1)}")
         print(f"Solution x=10 is now {new sol 2} with fitness {fitness(new sol 2)}")
        Solution x=1 is now 10 with fitness -5
        Solution x=10 is now 1 with fitness 22
In [250... pair3_1, pair3_2 = one_point_crossover("1011", "1100", 1)
         new_sol_1 = solution_dict[pair3_1]
         new_sol_2 = solution_dict[pair3_2]
         pair3 = [new_sol_1, new_sol_2]
         pair3_vectors = [pair3_1, pair3_2]
         print(pair3)
```

Solutions	Vector	Fitness
3	1000	30
1	0011	22
0	1011	15
9	1100	6
10	0101	- 5
12	0111	-33

===========

Total fitness: 35

Best solution: 3 with fitness 30

For pair 1, (x=15, x=6), one point crossover at position 1 created two new vectors, "0111" and "1000". These corresponded to the solutions 12 with fitness -33, and solution 3 with fitness 30.

For pair 2, (x=1, x=10), the one point crossover just resulted in them swapping, so (x=10, x=1). No new strings/solutions were created.

Finally, for pair 3, (x=0, x=9), the one point crossover changed x=0 into solution 9 with fitness 6, and changed x=9 into solution 0 with fitness 15; once again, no new vectors or solutions were created.

The fitness of the population did increase as a whole. The total fitness after crossing over was 35, while the previous population had a total fitness of -25.

The best solution also changed to be x=3 with a fitness of 30

2 d)

New pairs are generated from population c), pairing the best fit and least fit solutions:

```
In [282... # Sort c pop solutions
         c pop solutions.sort(key=fitness)
         d_pairs = generate_pairs(c_pop_solutions)
         print(d pairs)
        [(12, 3), (10, 1), (9, 0)]
In [283... d_pop_vectors = []
         for vector in c_pop_vectors:
             d_pop_vectors.append(mutate(vector, 3))
         print("Population d) vectors after mutating position 3 from population c)
        Population d) vectors after mutating position 3 from population c) is:
         ['0110', '1000', '0100', '0010', '1100', '1010']
In [284... # d_pair1_vectors = []
         # d_pair2_vectors = []
         # d pair3 vectors = []
         # d_pair1_solutions = []
         # d pair2 solutions = []
         # d_pair3_solutions = []
         # for vector in pair1 vectors:
               mutated vector = mutate(vector, 3)
               d_pair1_vectors.append(mutated_vector)
               d pair1 solutions.append(solution dict[mutated vector])
         # for vector in pair2_vectors:
               mutated vector = mutate(vector, 3)
               d pair2 vectors.append(mutated vector)
               d_pair2_solutions.append(solution_dict[mutated_vector])
         # for vector in pair3 vectors:
               mutated vector = mutate(vector, 3)
               d pair3 vectors.append(mutated vector)
               d pair3 solutions.append(solution dict[mutated vector])
         # print("New pair 1 for d): ", d_pair1_solutions, d_pair1_vectors)
         # print("New pair 2 for d): ", d_pair2_solutions, d_pair2_vectors)
         # print("New pair 3 for d): ", d_pair3_solutions, d_pair3_vectors)
In [285... | d_pop_solutions = [solution_dict[vector] for vector in d_pop_vectors]
         print("Population solutions from d) is: \n", d_pop_solutions)
         print("Population solutions from b) is: \n", pop)
         print("Population solutions from c) is: \n", c_pop_solutions)
        Population solutions from d) is:
         [11, 3, 8, 4, 9, 7]
        Population solutions from b) is:
         [15, 10, 9, 0, 1, 6]
        Population solutions from c) is:
         [12, 10, 9, 0, 1, 3]
```

In [286... evaluate_population(d_pop_solutions)

Solutions	Vector	Fitness
4	0010	31
3	1000	30
7	1010	22
8	0100	15
9	1100	6
11	0110	-18

Total fitness: 86

Best solution: 4 with fitness 31

We have new solutions after mutating population C. The new solutions are 11, 8, 4, and 7. These are solutions that have not appeared before in either Population C) or the original Population from B).

The fitness of solution 11 is -18. The fitness of solution 8 is 15. The fitness of solution 4 is 31, and the fitness of solution 7 is 22.

Mutation increased the total fitness of the population, as the total fitness is now 86. Mutation also found a better solution, as the best solution is now 4 with a fitness of 31, as opposed to the previous best fitness of 30.

Pairs were not really important in this step because only mutations occurred (pairs only relevant for crossing over)

2 e)

[9, 8, 7, 3, 4, 4]

```
Out [289... [(9, 4), (8, 4), (7, 3)]
In [300... # Perform 2 point cross over for each pair, exchanging the inner two element
         # point1 = 1, point2 = 3
         e_pop_vectors = []
         e_pop_solutions = []
         for pair in e pairs:
             print("Old Pair is: ", pair)
             vec1 = vector dict[pair[0]]
             vec2 = vector_dict[pair[1]]
             new_vec1, new_vec2 = two_point_crossover(vec1, vec2, 1, 3)
             e pop vectors.append(new vec1)
             e pop vectors.append(new vec2)
             solution1 = solution dict[new vec1]
             solution2 = solution_dict[new_vec2]
             e_pop_solutions.append(solution1)
             e pop solutions.append(solution2)
             print(f"New Pair is now: ({solution1}, {solution2})")
         print("Population e) vectors after two point crossing over of population d):
        Old Pair is: (9, 4)
        New Pair is now: (7, 8)
        Old Pair is: (8, 4)
        New Pair is now: (4, 8)
        Old Pair is: (7, 3)
        New Pair is now: (3, 7)
        Population e) vectors after two point crossing over of population d):
         ['1010', '0100', '0010', '0100', '1000', '1010']
In [302... print("Population solutions from b) is: \n", pop)
         print("Population solutions from c) is: \n", c_pop_solutions)
         print("Population solutions from d) is: \n", d_pop_solutions, "\n")
         print("Population solutions from e) is: \n", e_pop_solutions)
        Population solutions from b) is:
         [15, 10, 9, 0, 1, 6]
        Population solutions from c) is:
         [12, 10, 9, 0, 1, 3]
        Population solutions from d) is:
         [11, 9, 8, 7, 3, 4]
        Population solutions from e) is:
         [7, 8, 4, 8, 3, 7]
In [303... evaluate population(e pop solutions)
```

Solutions	Vector	Fitness
4	0010	31
3	1000	30
7	1010	22
7	1010	22
8	0100	15
8	0100	15

Total fitness: 135

Best solution: 4 with fitness 31

We don't have any brand new solutions, but after two point crossing over, pair (9,

4) has been replaced by pair (7, 8). The other stayed the same, but swapped places.

We have increased the total population fitness, as it is now 135 as opposed to the previous 86. We have already found the best solution of 4 with fitness 31

2 f)

```
In [293... # Sort the population from e) in ascending order by fitness
         e_pop_solutions.sort(key=fitness)
         e_pop_solutions
Out [293... [8, 8, 7, 7, 3, 4]
In [294... # Replace the least fit member with a clone of the best fit member
         f pop solutions = e pop solutions.copy()
          f_pop_solutions[0] = f_pop_solutions[len(f_pop_solutions)-1]
         f_pop_solutions
Out [294... [4, 8, 7, 7, 3, 4]
In [295... | # Generate pairs of best-fit and least-fit solutions
         f_pop_solutions.sort(key=fitness)
         print(f pop solutions)
         f_pairs = generate_pairs(f_pop_solutions)
         f_pairs
        [8, 7, 7, 3, 4, 4]
Out[295... [(8, 4), (7, 4), (7, 3)]
In [298... # Perform one point cross over for each pair, between the 3rd and 4th element
         # and exchange the first 3 elements of each pair
          f pop vectors = []
          f_pop_solutions = []
          for pair in f_pairs:
              print("Old Pair is: ", pair)
              vec1 = vector_dict[pair[0]]
              vec2 = vector dict[pair[1]]
              new_vec1, new_vec2 = one_point_crossover(vec1, vec2, 3)
```

```
f_pop_vectors.append(new_vec1)
             f_pop_vectors.append(new_vec2)
             solution1 = solution dict[new vec1]
             solution2 = solution_dict[new_vec2]
             f pop solutions.append(solution1)
             f pop solutions.append(solution2)
             print(f"New Pair is now: ({solution1}, {solution2})")
         print("Population f) vectors after one point crossing over between 3rd and 4
         # Population d) vectors ['1010', '0100', '0010', '0100', '1000', '1010']
        Old Pair is: (8, 4)
        New Pair is now: (8, 4)
        Old Pair is: (7, 4)
        New Pair is now: (7, 4)
        Old Pair is: (7, 3)
        New Pair is now: (7, 3)
        Population f) vectors after one point crossing over between 3rd and 4th elem
        ent of population e):
         ['1010', '0100', '0010', '0100', '1000', '1010']
In [299... print("Population solutions from b) is: \n", pop)
         print("Population solutions from c) is: \n", c_pop_solutions)
         print("Population solutions from d) is: \n", d_pop_solutions)
         print("Population solutions from e) is: \n", e_pop_solutions, "\n")
         print("Population solutions from f) is: \n", f_pop_solutions)
        Population solutions from b) is:
         [15, 10, 9, 0, 1, 6]
        Population solutions from c) is:
         [12, 10, 9, 0, 1, 3]
        Population solutions from d) is:
         [11, 9, 8, 7, 3, 4]
        Population solutions from e) is:
         [8, 8, 7, 7, 3, 4]
        Population solutions from f) is:
         [8, 4, 7, 4, 7, 3]
In [305... evaluate_population(f_pop_solutions)
        Solutions
                     Vector
                                  Fitness
        4
                     0010
                                   31
        4
                     0010
                                   31
        3
                     1000
                                   30
        7
                     1010
                                   22
        7
                                   22
                     1010
                     0100
                                   15
        Total fitness: 151
        Best solution: 4 with fitness 31
```

No brand new solutions were generated, and no new solutions were generated from crossing-over. However, deleting the least fit solution 8 and replacing it with

another 4 increased the total population fitness from 135 to 141. We already found the best solution of 4 with fitness 31, so we did not improve upon that.

2 g)

The encoding of the solution space was adequate. This is because crossing-over did not tend to lose the positive characteristics of the most fit solutions, while also introducing diversity into lesser fit solutions to make them more fit. A great example of this is in f), where crossing over between the 3rd and 4th elements did not cause any of the already very fit solutions to be lost, but instead simply swapped their positions in the pair. Thus, this encoding is adequate for Genetic Algorithms, as it allows the introduction of diversity for lesser fit solutions while retaining the best fitness solutions. Eventually the lesser fit solutions are competed out by the best fitness solutions, ala Darwin's theory of natural selection.