Assignment 4

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Simulated Annealing

Importing relevant packages

In [1]:

```
import random
import matplotlib.pyplot as plt
import math
```

Returns a random motif of given length

In [2]:

```
def random_motif(length_motif):
    motif = ""
    n = ["a", "t", "c", "g"]
    for i in range(length_motif):
        motif += random.choice(n)
    return motif
```

Hamming score returns score equal to the number of matching nucleotides in 2 sequences, more the similarity higher the score

In [3]:

```
def hamming_score(s1, s2):
    sc = 0
    for i in range(len(s1)):
        if s1[i] == s2[i]:
            sc += 1
    return sc
```

Cost function to maximise score and return it This calculates score by fiding max hamming score for each sequence and then adding scores for all sequences

In [4]:

```
def cost_function(list_dna, motif):
    cum_score = 0
    length_motif = len(motif)
    for dna in list_dna:
        score = 0
        for ind in range(len(list_dna[0])-length_motif+1):
            score = max(score, hamming_score(motif, dna[ind: ind+length_motif]))
            # print("ham", motif, dna[ind: ind+length_motif])
        cum_score += score
        # maximise cumulative score
    return cum_score
```

find_neighbour returns a sequence with max 2 mutations

In [5]:

```
def find_neighbour(motif):
    # max 2 mutations
    pos1 = random.randint(0, len(motif)-1)
    pos2 = random.randint(0, len(motif)-1)
    motif = motif[:pos1] + random.choice(["a", "t", "c", "g"]) + motif[pos1 + 1:]
    motif = motif[:pos2] + random.choice(["a", "t", "c", "g"]) + motif[pos2 + 1:]
    return motif
```

Function that performs simulated annealing

Calls functions to find random motif, calculates its cost and while conditions are favorable, keeps finding neighbours and updating scores, changes t every iteration

Runs for maximum 500 iterations if loop doesn't break

Finds best motif match and prints it

Also plots a graph to show costs and iterations

In [6]:

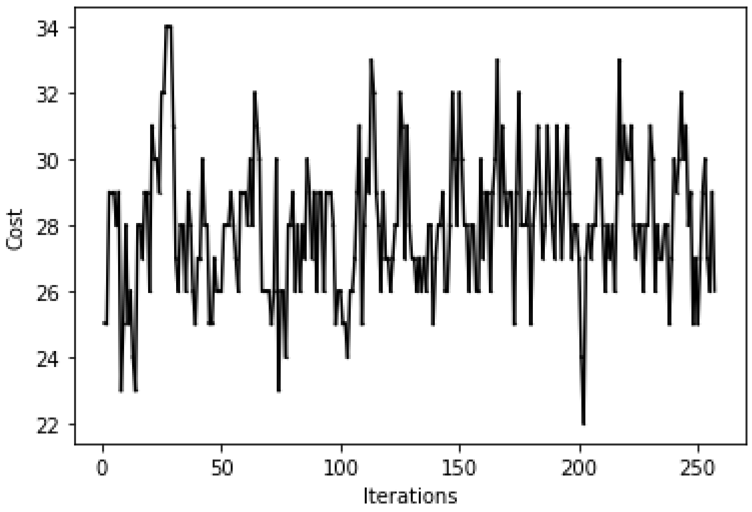
```
def simulated_annealing(list_dna, length_motif):
    motif = random_motif(length_motif)
    cost_new = cost_function(list_dna, motif)
    cost_old = 0
    final_motif = ""

    plt.xlabel('Iterations')
    plt.ylabel('Cost')
    time = 1
    flag = True
    iterations = 0
    t = 2000
    while flag:
        # print(cost_new, motif)
        iterations += 1
        plt.plot(time, cost_new, color='black', marker='o', markersize=0.3)
        time += 1
        neighbour = find_neighbour(motif)
        cost_old = cost_new
        cost_new = cost_function(list_dna, neighbour)
        max_cost = 0
        if cost_new > max_cost:
            max_cost = cost_new
            final_motif = motif

        if iterations > 500:
            flag = False

        elif cost_new >= cost_old:
            motif = neighbour

        else:
            try:
                # probability of e^(-cost/t)
                if random.uniform(0, 1) < math.exp(-(cost_new - cost_old) / t):
                    motif = neighbour

            except:
                flag = False


        t *= 0.95

    # plt.plot(time, cost_new, color='black', marker='o', markersize=3)
        plt.plot([time-1, time], [cost_old, cost_new], 'k-')


    plt.show()
    return final_motif
```

Main Function to take inputs

In [7]:

```
if __name__ == "__main__":
    list_dna = []
    length_motif = int(input("Enter length: "))
    no_of_seq = int(input("Enter no of seq: "))
    for i in range(no_of_seq):
        list_dna.append(input())
    ans = simulated_annealing(list_dna, length_motif)
    print(ans)
```

```
Enter length: 10
Enter no of seq: 5
agcaatcgcccgtattccgttaaagcctgcctcgctagctcgaagctg
ggtcttgcgtgcatcgctaagctagcaaccgctagcatgcgctagcct
gattcgaataggcaaacgcacgaagtccgttaaagctagcatcgatcg
gctagctagcactattccgttttagcgatccgcctagccagagagatc
ccgctcgatcgtagcggatcgctagcatttcgttatccgtgcatagcg
```



```
taaagttaca
```

So the best match is found to be: taaagttaca