

Optimization Methods/Meta-Heuristics

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Abstract. This paper explores the TRAVELLING SALESMAN PROBLEM. This problem (also called the travelling salesperson problem or TSP) asks the following question: "Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?". Hill-climbing, simulated annealing, tabu search and genetic algorithms were used to analyze the best route for different sets of cities.

1 Specification of the Work Performed

1.1 Practical work topic

The project goal is to answer the practical work Topic 3: Metaheuristics for Optimization/Decision Problems. As indicated in the practical work paper, "an optimization problem is characterized by the existence of a (typically large) set of possible solutions, comparable to each other, of which one or more are considered (globally) optimal solutions. Depending on the specific problem, an evaluation function allows you to establish this comparison between solutions. In many of these problems, it is virtually impossible to find the optimal solution, or to ensure that the solution found is optimal and, as such, the goal is to try to find a local optimal solution that maximizes/minimizes a given evaluation function to the extent possible".^[1]

1.2 Problem definition

Our team choose to study the TRAVELLING SALESMAN PROBLEM. This problem (also called the travelling salesperson problem or TSP) asks the following question: "Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?".

The problem was first formulated (mathematically) in 1930 and is one of the most intensively studied problems in optimization. It is used as a benchmark for many optimization methods. Even though the problem is computationally difficult, many heuristics and exact algorithms are known, so that some instances with tens of thousands of cities can be solved completely and even problems with millions of cities can be approximated within a small fraction of 1%.

The TSP has several applications even in its purest formulation, such as planning, logistics, and the manufacture of microchips. Slightly modified, it appears as a sub-problem in many areas, such as DNA sequencing. In these applications, the concept city represents, for example, customers, soldering points, or DNA fragments, and the concept distance represents travelling times or cost, or a similarity measure between DNA fragments. The TSP also appears in astronomy, as astronomers observing many sources will want to minimize the time spent moving the telescope between the sources; in such problems, the TSP can be embedded inside an optimal control problem. ^[2]

This problem is easy to declare but very difficult to solve. When completed in exact time the required computation will increase exponentially as the problem increases.

TSP can be expressed as a problem in finding the minimum distance of a closed journey to a number of n cities where the cities are only visited once. TSP is represented by using a complete and weighted graph $G = (V, E)$ with V set of vertices representing a set of points, and E is the set of edges. Each edge $(r, s) \in E$ is the value (distance) r_s which is the distance from city r to city s , with $(r, s) \in V$. In a symmetric TSP (distance from city r to point s is equal to distance from point S to point r), $d_{rs} = d_{sr}$ for all edges $(r, s) \in E$. In a graph, the TSP is drawn as shown in Figure 1 below: ^[3]

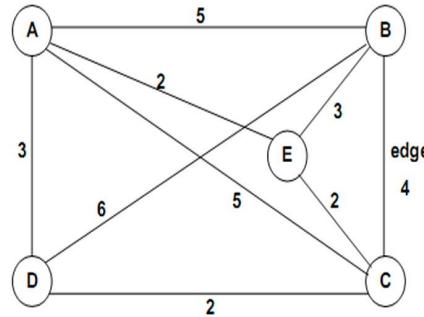


Fig.1 – The illustration of TSP

2 Related Works

There are lots of papers, articles and thesis regarding the TSP. We used some of these texts as a guide for our work. We also used the slides presented by the teacher in the classroom.

We do not intend to create new technologies in this work, but to use best practices. That's why we highlight below the best definitions we found, indicating the authors.

2.1 Hill-Climbing

“Hill climbing is a mathematical optimization algorithm, which means its purpose is to find the best solution to a problem which has a (large) number of possible solutions. In the Travelling salesman problem, the distances between each pair of cities are known, and we need to find the shortest route. The goal is to find the best (i.e. the shortest) solution. It tries to find the best solution to this problem by starting out with a random solution, and then generate neighbours: solutions that only slightly differ from the current one. If the best of those neighbours is better (i.e. shorter) than the current one, it replaces the current solution with this better solution. It then repeats the pattern by again creating neighbours. If at some point no neighbour is better than the current solution, it returns the then current solution”. [4]

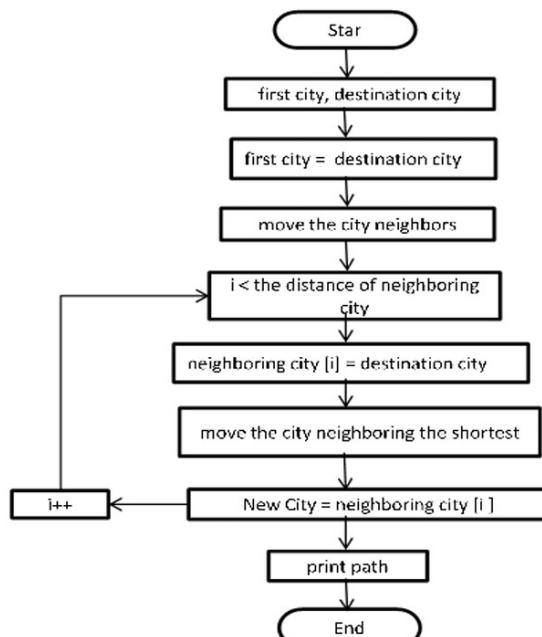


Fig.2 – Hill-Climbing flowchart [3]

2.2 Simulated Annealing

“The Simulated Annealing (SA) approach begins with a random solution and every iteration forms a random closely solution. If the closely solution is an over top answer, it would substitute by the present solution, but if it is a worsen answer, it may be chosen to substitute the present solution with a probability that will be dependent on the temperature variable (parameter). As the approach continues, the temperature variable (parameter) reduces, thus giving worse answer a lower chance of substituting the present

answer. Allowing worse answers assists to stay away from converging to a local minimum rather than the global minimum". [5]

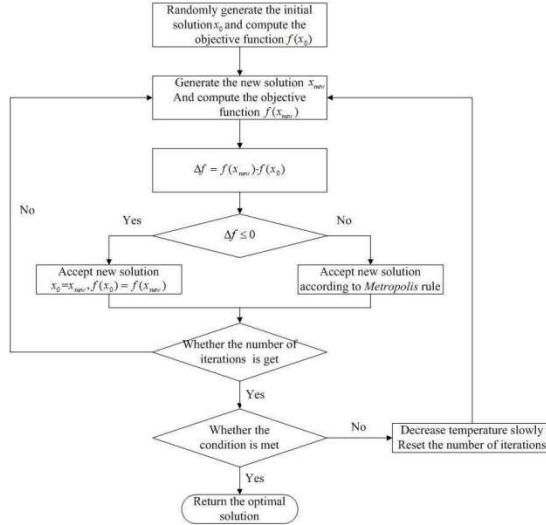


Fig.3 – Simulated Annealing flowchart [6]

2.3 Tabu Search

“Tabu Search is a Global Optimization algorithm and a Metaheuristic for controlling an embedded heuristic technique. Tabu Search algorithm is to force an embedded heuristic from returning to recently visited areas of the search space, which is called as cycling. The plan of this approach is to maintain a temporary memory for all the changes of recent moves within the search space and preventing future moves from undoing those changes. In addition to this, an intermediate memory will be used for other search spaces. Tabu search is based on local search. The search starts with an initial solution for the problem. That initial solution is taken as a current solution and searches for the best solution i.e. a group of tours that can be simply reached from the current solution. After this step, it takes the best solution from the neighborhood as the current solution and the search process continues. Tabu search is terminated when it meets the maximum iteration count conditions, solution quality objectives or involving in the execution time”. [7]

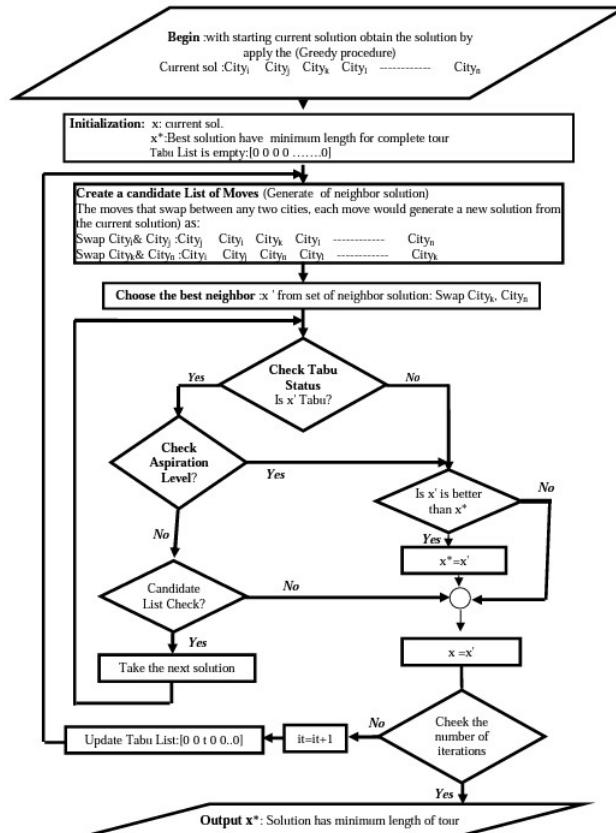


Fig.4 – Tabu Search flowchart [8]

2.4 Genetic Algorithms

“Genetic Algorithm (GA) is a search-based algorithm inspired by Charles Darwin’s theory of natural evolution. GA follows the notion of natural selection. The process of natural selection starts with the selection of fittest individuals from a population. They produce offspring which inherit the characteristics of the parents and will be added to the next generation. If parents have better fitness, their offspring will be better than parents and have a better chance at surviving. This process keeps on iterating and at the end, a generation with the fittest individuals will be found. We can use this notion for search-based algorithm. We can formally state this process in as following phases: 1. Initial population, 2. Fitness Function, 3. Selection, 4. Cross-over and 5. Mutation.” [9]

“Genetic algorithms appear to find good solutions for the traveling salesman problem, however it depends very much on the way the problem is encoded and which crossover and mutation methods are used”. [10]

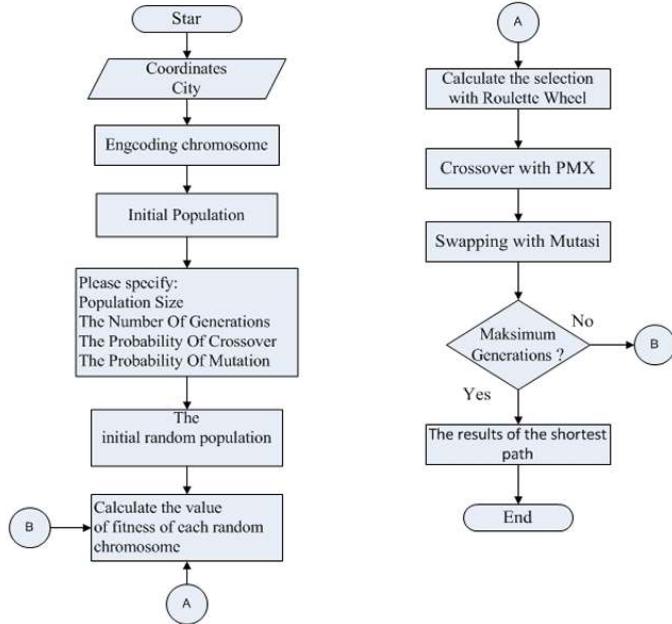


Fig. 5 – Genetic Algorithms flowchart [3]

2.5 Solving Optimization Problems

“Heuristic algorithms do not guarantee to find the optimal solution and do not have a bound on quality, that is, they can return a solution that is arbitrarily bad compared to the optimal solution. However, in practice, heuristic algorithms (heuristics for short) have proven very successful in solving large real-world problems”. [11]

3 Formulation of the Problem as an Optimization Problem

The idea of the TSP is to find a tour of a given number of cities/locations, visiting each of them exactly once and returning to the starting city/location where the length of this tour is minimized.

In this work, hill-climbing, simulated annealing, tabu search and genetic algorithms have been used to analyze the best route and the time spent to process the solution for the following sets:

- **4 x 4 matrix (used for testing):** travel between Porto, Braga, Aveiro and Viana do Castelo.
- **14 x 14 matrix:** travel between Lisboa, Porto, Braga, Setubal, Coimbra, Evora, Aveiro, Leiria, Faro, Viana do Castelo, Beja, Braganca, Castelo Branco and Guarda.
- **37 x 37 matrix:** travel between Amsterdam, Antwerp, Athens, Barcelona, Berlin, Bern, Brussels, Calais, Cologne, Copenhagen, Edinburgh, Frankfurt, Geneva, Genoa, Hamburg, Le Havre, Lisbon, London, Luxembourg, Lyon, Madrid, Marseille, Milan, Munich, Naples, Nice, Paris, Prague, Rome, Rotterdam, Strasbourg, Stuttgart, The Hague, Turin, Venice, Vienna and Zurich.

Those datasets were obtained at the website <https://pt.melhoresrotas.com/> [12] for the Portuguese cities and in <https://www.engineeringtoolbox.com/> [13] for the European cities. Latitude and longitude data were found at the web site <https://simplemaps.com/> [14]. More details could be found in the python notebook presented as part of this work.

We aim to present a comparative study among those algorithms for solving TSP. Some algorithms have not found a better solution to the traveling salesman problem than is already known. It is very difficult to say that what moderate sized instance is unsolvable, so an incorporation of good local search technique to the algorithm may solve exactly the other instances, which is under our investigation and is categorized under future work.

4 Implementation Details

All the work has been developed in Python, using the Jupyter Notebook (anaconda3) to run the program. The following libraries has been used: numpy, pandas, gmplot, time, random, math, matplotlib, copy, sys, datetime, warnings, sys, random, copy and `dataframe_image`.

The datasets used were obtained at the internet, see references [12], [13] and [14].

The results presented were obtained on a desktop with the following configurations:

- MS Windows 10 Pro OS – Version 10.0.19043 Build 19043 • System type X64-based PC • Intel(R) Core (TM) i7-4771 CPU @ 3.50GHz, 3501Mhz, 4 Cores, 8 Processors
- BIOS Version/Date American Megatrends Inc. 3503, 4/18/18 • BaseBoard GRYPHON Z97 ARMOR EDITION (ASUS) • Memory (RAM) 32.0 GB • Graphics Card NVIDIA GeForce GTX 1650 4Gb.

5 Approach and Algorithms Implemented

All selected algorithms were executed with 500, 1.000, 5.000 and 10.000 iterations. The specific functions of each algorithm, such as stopping criteria, evaluation functions and other operators are shown below.

5.1 Hill-Climbing:

Hill climbing tries to find the best solution to this problem by starting out with a random solution, and then generate neighbours: solutions that only slightly differ from the current one. If the best of those neighbours is better (i.e. shorter) than the current one, it replaces the current solution with this better solution. It then repeats the pattern by again creating neighbours. If at some point no neighbour is better than the current solution, it returns the then current solution.

- Iterations: 500, 1.000, 5.000 and 10.000.
- Neighborhood: random swap among two neighbors.
- Mutation rate: (optional), a number, from 0.00 to 1.00. Randomly discards neighbors depending on the chosen rate, with 1 being equivalent to not discarding any. (mutation_rate = 0.7, i.e discarding 30% of the neighbors).

STEP 1: Hill-Climbing starts generating a random solution, so we define a function to create a random solution generator.

```
def get_random_solution(matrix:[], home:int, city_indexes:[])
    # Create a list with city indexes
    cities = city_indexes.copy()
    # Remove the home city
    cities.pop(home)
    # Create a population
    population = []
    for i in range(size):
        # Shuffle cities at random
        random.shuffle(cities)
        # Create a state
        state = State(cities[:])
        state.update_distance(matrix, home)
        # Add an individual to the population
        population.append(state)
    # Sort population
    population.sort()
    # Return the best solution
    return population[0]
```

STEP 2: We want our Hill climber to find the shortest solution, so we need a function calculating the length of a specific solution.

```

# Update distance
def update_distance(self, matrix, home):

    # Reset distance
    self.distance = 0
    # Keep track of departing city
    from_index = home
    # Loop all cities in the current route
    for i in range(len(self.route)):
        self.distance += matrix[from_index][self.route[i]]
        from_index = self.route[i]
    # Add the distance back to home
    self.distance += matrix[from_index][home]

```

STEP 3: Create a function to defining neighbors. To make our hill climbing less greedy we can randomly select among neighbors, discarding some. Setting value to 1 or greater deactivate the function.

```

# Mutate a solution
def mutate(matrix:[], home:int, state:State, mutation_rate:float=0.01):

    # Create a copy of the state
    mutated_state = state.deepcopy()
    # Loop all the states in a route
    for i in range(len(mutated_state.route)):
        # Check if we should do a mutation
        if(random.random() < mutation_rate):
            # Swap two cities
            j = int(random.random() * len(state.route))
            city_1 = mutated_state.route[i]
            city_2 = mutated_state.route[j]
            mutated_state.route[i] = city_2
            mutated_state.route[j] = city_1
    # Update the distance
    mutated_state.update_distance(matrix, home)
    # Return a mutated state
    return mutated_state

```

STEP 4: Create a function finding the best neighbour. The best solution is mutated in each iteration and a mutated solution will be the new best solution if the total distance is less than the distance for the current best solution.

```

# Get best solution by distance
def get_best_solution_by_distance(matrix:[], home:int):

    # Variables
    route = []
    from_index = home
    length = len(matrix) - 1
    # Loop until route is complete
    while len(route) < length:
        # Get a matrix row
        row = matrix[from_index]
        # Create a list with cities
        cities = {}
        for i in range(len(row)):
            cities[i] = City(i, row[i])
        # Remove cities that already is assigned to the route
        del cities[home]
        for i in route:
            del cities[i]
        # Sort cities
        sorted = list(cities.values())
        sorted.sort()
        # Add the city with the shortest distance
        from_index = sorted[0].index
        route.append(from_index)
    # Create a new state and update the distance
    state = State(route)
    state.update_distance(matrix, home)
    # Return a state
    return state

```

STEP 5: Hill climbing algorithm creates a random solution and calculate its route length. We then create the neighbouring solutions, and find the best one. From there on, as long as the best neighbour is better than the current solution, we repeat the same pattern with the current solution each time being updated with the best neighbour. When this process stops, we return the current solution (and its route length).

```
# Setting mutation rate:
mut_rate = 0.7

# Hill climbing algorithm
def hill_climbing(matrix:[], home:int, initial_state:State, max_iterations:int, mutation_rate:float=0.01):
    # Keep track of the best state
    best_state = initial_state
    # An iterator can be used to give the algorithm more time to find a solution
    iterator = 0
    #list row
    row = []
    # Create an infinite loop
    while True:
        # Mutate the best state
        neighbor = mutate(matrix, home, best_state, mutation_rate)
        # Check if the distance is less than in the best state
        if(neighbor.distance >= best_state.distance):
            iterator += 1
            if (iterator >= max_iterations):
                break
        if(neighbor.distance < best_state.distance):
            best_state = neighbor
            row = row + [[iterator,neighbor.distance]]
    # Return the best state
    return best_state, row
```

STEP 6: At the end, we define the function to run with our dataset getting the solution.

```
#Get time of processing
start_time = time.time()

# Distances in km between cities, same indexes (i, j) as in the cities array
matrix = cities4_4_hill_climbing
# Cities to travel
cities = ['Porto', 'Braga', 'Aveiro', 'Viana do Castelo']
city_indexes = [0,1,2,3]

# Index of start location
home = random.randrange(0,4)

# Max iterations
max_iterations = num_inter

# Distances in km between cities, same indexes (i, j) as in the cities array
matrix = cities4_4_hill_climbing

# Run hill climbing to find a better solution
state = get_best_solution_by_distance(matrix, home)
state,iterations = hill_climbing(matrix, home, state, max_iterations, mut_rate)

print('-- Hill climbing solution --')
print(cities[home], end='')
df = [cities[home]]
for i in range(0, len(state.route)):
    print(' -> ' + cities[state.route[i]], end='')
    df.append(cities[state.route[i]])
print(' -> ' + cities[home], end='')
df.append(cities[home])
print('\n\nTotal distance: {} km'.format(state.distance))
print()

#time
hill_teste_time = time.time() - start_time
print("... %s seconds ..." % (hill_teste_time))
```

Stopping criteria's of Hill-Climbing algorithm is:

- The algorithm performed all the maximum iterations established.

5.2 Simulated Annealing:

The Simulated Annealing algorithm is commonly used when we're stuck trying to optimize solutions that generate local minimum or local maximum solutions, for example, the Hill-Climbing algorithm.

- Iterations: 500, 1.000, 5.000 and 10.000.
- Cooling schedule: Initial temperature: sated to 1000° / Final temperature: 0° / Rate: ~0.005. The temperature is a parameter that affects two aspects of the algorithm: (a) The distance of a trial point from the current point and (b) The probability of accepting a trial point with higher objective function value.
- Neighborhood: random swap among two neighbors.
- Mutation rate: (optional), a number, from 0.00 to 1.00. Randomly discards neighbors depending on the chosen rate, with 1 being equivalent to not discarding any. (mutation_rate = 0.7, i.e discarding 30% of the neighbors).

STEPS 1 to 4: The same we use for Hill-Climbing.

STEP 5: We have to determine how we will reduce the temperature on each iteration. We started with a temperature of 1000 degrees, and we will decrease the current temperature at a -0,5% rate trying to reach the final temperature of 0 degrees. We will repeat this process until the current temperature is less than the final temperature.

```
# Setting mutation rate and temperature:
mut_rate = 0.5
initial_temp = 1000
# Schedule function for simulated annealing
def exp_schedule(k=initial_temp, lam=0.005, limit=num_inter):
    return lambda t: (k * np.exp(-lam * t)) if t <= limit else 0
```

STEP 6: If the new solution is better, we will accept it, but if the new solution is not better, we will still accept it if the temperature is high. With this approach, we will use the worst solution in order to avoid getting stuck in local minimum. But we will get a neighbor that is not much worse than the current state. We can determine defining these functions:

```
# Return true with probability p
def probability(p):
    return p > random.uniform(0.0, 1.0)

# Calculate the change in e
delta_e = best_state.distance - neighbor.distance
# Check if we should update the best state
if delta_e > 0 or probability(np.exp(delta_e / T)):
    best_state = neighbor
```

STEP 7: This is the big picture for Simulated Annealing algorithm, which is the process of taking the problem and continuing with generating random neighbors. We'll always move to a neighbor if it's better than our current state. But even if the neighbor is worse than our current state, we'll sometimes move there depending on the temperature and how bad the neighbor is. Finally, we stop if the maximum iteration has been reached.

```
# Setting mutation rate and temperature:
mut_rate = 0.7
initial_temp = 1000

# Return true with probability p
def probability(p):
    return p > random.uniform(0.0, 1.0)

# Schedule function for simulated annealing
def exp_schedule(k=initial_temp, lam=0.005, limit=num_iter):
    return lambda t: (k * np.exp(-lam * t)) if t <= limit else 0

# Simulated annealing
def simulated_annealing(matrix: [], home:int, initial_state:State, mutation_rate:float=0.01, schedule=exp_schedule()):
    # Keep track of the best state
    best_state = initial_state
    #list row
    row = []
    # Loop a Large number of times (int.max)
    for t in range(sys.maxsize):
        # Get a temperature
        T = schedule(t)
        # Return if temperature is 0
        if T == 0:
            return best_state, row
        # Mutate the best state
        neighbor = mutate(matrix, home, best_state, mutation_rate)
        # Calculate the change in e
        delta_e = best_state.distance - neighbor.distance
        # Check if we should update the best state
        if delta_e > 0 or probability(np.exp(delta_e / T)):
            best_state = neighbor
        row = row + [[t, neighbor.distance, T]]
    # Return the best state
    return best_state, row
```

STEP 8: At the end, we define the function to run with our dataset getting the solution.

```
#Get time of processing
start_time = time.time()

# Cities to travel
cities = ['Porto', 'Braga', 'Aveiro', 'Viana do Castelo']
city_indexes = [0,1,2,3]
# Index of start location
home = random.randrange(0,4)
# Distances in miles between cities, same indexes (i, j) as in the cities array
matrix = cities4_4_simulated_annealing

# Run simulated annealing to find a better solution
state = get_best_solution_by_distance(matrix, home)
state = simulated_annealing(matrix, home, state, mut_rate)
print('-- Simulated annealing solution --')
print(cities[home], end='')
df = [cities[home]]
for i in range(0, len(state.route)):
    print(' -> ' + cities[state.route[i]], end='')
    df.append(cities[state.route[i]])
print(' -> ' + cities[home], end='')
df.append(cities[home])
print('\n\nTotal distance: {} km'.format(state.distance))

#time
SimuAnnealing_teste_time = time.time() - start_time
print("---- %s seconds ----" % (SimuAnnealing_teste_time))
```

Stopping criteria's of simulated annealing algorithm are:

- The algorithm performed all the maximum iterations established.
- A given minimum value of the temperature has been reached.

5.3 Tabu Search:

Tabu search uses a local or neighborhood search procedure to iteratively move from a solution to another solution until some stopping criterion has been satisfied. The aim is to explore regions of the search space that would be left unexplored by the local search procedure. Tabu search modifies the neighborhood structure of each solution as the search progresses. This metaheuristic guarantees a near optimal solution, using the concept of short term of memory space.

- Iterations: 500, 1.000, 5.000 and 10.000.
- Tabu tenure: the duration for which a move will be kept tabu. This parameter is selected depending on the size n of the problem by the algorithm $T=\sqrt{n}$
 - 4 x 4 matrix = 2 iterations
 - 14 x 14 matrix = 4 iterations
 - 37 x 37 matrix = 6 iterations
- Neighborhood: identify neighborhood set by creating many solutions with move operation
 - 4 x 4 matrix = 1
 - 14 x 14 matrix = 1
 - 37 x 37 matrix: = 1

STEP 1: Tabu search is based on local search, which starts with an initial solution for the problem. That initial solution is taken as a current solution and searches for the best solution, in which a group of tours that can be simply reached from the current solution. After this step, it takes the best solution from the neighborhood as the current solution and the search process continues. With the sample project datasets, the algorithm starts with a range from 1 to the length of all the cities of the matrices plus one.

Input the number of cities (data), and the distances between them.

```
#Data
data = cities4_4.reset_index()
```

The *solution variable* is the initial solution, which is taken as a current solution

```
# Current solution initialization
solution = list(range(1, len(data) + 1)) # List of all job indexes from the file
```

Tabu search is terminated when it meets the maximum iteration count conditions, solution quality objectives or involving in the execution time. Therefore, the algorithm uses three parameters.

Parameter 1: Iterations (iterations) is the number of times that the current solution will be reevaluated with the goal of finding a better optimal solution. Criteria for stopping the algorithm after several iterations.

Parameter 2: Tabu length (*tabu_len*) keeps the last solution for a specific number of new interactions. This is usually obtained by keeping track of the last solutions in terms of the action used to transform one solution to the next. When an action is performed it is considered tabu for the next T iterations, where T is the tabu status length.

T {is number of iterations for move will be kept tabu where $t = \sqrt{n}$ }

Parameter 3: Identify Neighborhood set by creating many solutions with used move operation. The move operation in the TSP is making swap between two cities or n number of cities randomly of the current solution.

```
# Setting of the stop criterion
iterations = num_inter # Parameter 1
tabu_len = 2 # Parameter 2 (sqrt(n))
neighbourhood = 1 #Parameter 3
```

STEP 2: Define the current solution as the best solution in the variable (*solution*). After it, calculate the aspiration level with the function (*count_score*). To be the first benchmark used inside the loop iteration. Aspiration criterion is used to override the tabu list when there is a good tabu move aspiration criterion. So, the tabu move is accepted if during the iterations, it produces better solution than the best obtained so far.

```
# Current solution initialization
solution = list(range(1, len(data) + 1)) # List of all job indexes from the file

# Creating array in order to conduct goal function calculations
m = np.delete(data.to_numpy(), 0, 1) # The first arrays column removal, because it contains indexes

# Solution Score
score = count_score(solution)
```

Also, we define three list for the looping processes:

- Tabu: Final list with the best possible route found.
- Candidates: Store the candidates list for evaluation. List used in the candidates_generator function.
- Scores_Tabu_teste: Store the evaluation scores of the new solutions inside the loop. Important for the concept of short term of memory space.

```

# Tabu List initialization
tabu = [] # Tabu List

# Creation of a candidate list of neighbors to the current solution
candidates = [] # A list of all candidates
scores_tabu_teste = []

```

Function *count_score* will calculate the total distance of the current route found by the algorithm.

```

def count_score(o): # Function responsible for counting score
    time_travel, copied_solution = 0, o.copy()
    time_travel = np.double(time_travel)
    for i in range(0, len(m) - 1):
        first_city, second_city = copied_solution[i], copied_solution[i + 1]
        time_travel += m[first_city - 1, second_city - 1]
    time_travel += m[copied_solution[0] - 1, copied_solution[-1] - 1]
    return time_travel

```

STEP 3: At this point, the while stop criterion loop starts, in order to find the best possible solution. Inside the looping, the algorithm uses two more defined functions, such as *candidates_generator* and *swap_method*.

Firstly, the while loop generates candidates, identifying neighborhood set by creating many solutions with used move operation. If the move is considered, it is held in the list until it moves is done and a new score is set. The move operation in TSP is making swap between any two cities randomly on the current solution.

```

def candidates_generator(n): # The function generating all candidates
    k, x, y = 0, 0, 0
    for k in range(0, neighbourhood):
        while True:
            while True:
                x, y = choice(n), choice(n)
                if x != y:
                    break
            if [x, y] not in candidates:
                candidates.append([x, y]) # Populating list with small lists of two numbers
                break
        k += 1

```

The *swap_method* function is responsible for changing positions in the list. It replaces a selected distance between two cities by another distance.

```

def swap_method(t1, y): # The first type of neighbourhood
    x = solution.index(t1)
    copied_solution = new_solution.copy() # Copied solution which is used for experiments
    copied_solution[x], copied_solution[y] = copied_solution[y], copied_solution[x] # Swapping positions of these jobs in neighbourhood
    neighbourhood_type = "swap"
    return copied_solution, neighbourhood_type

```

Swapping the positions, means that a new solution with a different score was generated by the function. Therefore, if the new score (total distance) is lower than the previous, the new value will be stored as a new current solution. Otherwise, it will check tabu length for preparing a new candidate list for the next iteration.

```

#Generate Solution
i = 0
while i != iterations:
    z = candidates_generator(solution) # Generating candidates
    min_solution, min_score = solution.copy(), score
    tabu_pair = [] #If the move is considered it is held in this List until it move is done and a new score is set

    j = 0
    while j != neighbourhood: # checking neighbourhood
        pair, new_solution, new_score = candidates[j].copy(), solution.copy(), 0 #candidates_score[j]
        if pair not in tabu:
            t1 = pair[0]
            y = new_solution.index(pair[1])
            new_solution, neighbourhood_type = swap_method(t1, y)
            new_score = count_score(new_solution)
            #Get distances
            scores_tabu_teste.append(min_score)
            if new_score < min_score: # Checking if a new score is better than local score
                min_solution, min_score, tabu_pair = new_solution.copy(), new_score, pair.copy()

            j += 1
            if min_score < score: # Checking if Local score can replace previous score
                solution, score = min_solution.copy(), min_score
                tabu.append(tabu_pair)
        if len(tabu) == tabu_len: # Controlling the tabu List Length
            del tabu[0]
            candidates.clear() # Preparing candidates list for the next iteration
        i += 1
    print("The results of Tabu Search algorithm for Teste")
    print("Solution: {solution}")

#Time
tabu_teste_time = time.time() - start_time
print("...%s seconds ..." % (tabu_teste_time))

```

Stopping criteria's of tabu search algorithm are:

- Overused resources as money, time, and computation.
- The algorithm seems unable to find something better and the current solution satisfies the requirements.
- Maximum iteration count conditions.
- Solution quality objectives.
- Maximum execution time.

5.4 Genetic Algorithms:

- Iterations: 500, 1.000, 5.000 and 10.000
- names_list: list of cities used in genesis functions to generate randomly population routes
 - 4 x 4 matrix
 - 14 x 14 matrix
 - 37 x 37 matrix
- n_cities: length of cities in each matrix
 - 4 x 4 matrix = 4
 - 14 x 14 matrix = 14
 - 37 x 37 matrix = 37

- `n_population`: number of populations that will be generated in `genesis` function by the initial progenitor (`n_population = 50`)
- `mutation_rate`: Defines the percentage of progenitors that will be mutate for a new evaluation. (`mutation_rate = 0.3`)

```
#Data transformation
names_list = list(cities4_4)
names_list = np.array(names_list)

#Parameters
#number of cities
n_cities = len(cities4_4)
#Population generated
n_population = 100
#mutation rate of progenitors
mutation_rate = 0.1
```

At firstly, the algorithm uses the `genesis` function to randomly defines N possible solutions to the problem. It doesn't need to be the best, because they will be the seed upon which later the best solution will be found.

```
#define population set
population_set = genesis(names_list, n_population)
```

`Genesis` function creates a loop with `n_population` to generate randomly new route solutions.

```
# First step: Create the first population set
def genesis(city_list, n_population):

    population_set = []
    for i in range(n_population):
        #Randomly generating a new solution
        sol_i = city_list[np.random.choice(list(range(n_cities)), n_cities, replace=False)]
        population_set.append(sol_i)
    return np.array(population_set)
```

After generating a set of N possible solutions, the algorithm uses a `fitness` function to evaluate each of the route individually and access one by one.

```
#define fitness list
fitnes_list = get_all_fitnes(population_set,cities_dict)
```

Fitness is a metric that represents how well each of the individual solutions performs for our model. In travel salesman problem, the algorithm is looking for the best possible route, which it means a minimization procedure. Therefore, the lowest fitness values return the best possible routes.

```
#define fitness list
def get_all_fitness(population_set, cities_dict):
    fitness_list = np.zeros(n_population)

    #Looping over all solutions computing the fitness for each solution
    for i in range(n_population):
        fitness_list[i] = fitness_eval(population_set[i], cities_dict)

    return fitness_list
def fitness_eval(city_list, cities_dict):
    total = 0
    for i in range(n_cities-1):
        a = city_list[i]
        b = city_list[i+1]
        total += compute_city_distance_names(a,b, cities_dict)
    return total
```

Fitness evaluation uses city distance names function, which demands latitude and longitude data to determinate the real distance between points. For each point in the population, a fitness value will be generated.

```
# List of coordinates representing each city
lat = cities4_4.latitude
lon = cities4_4.longitude
coordinates_list = [[x,y] for x,y in list(zip(lat,lon))]
cities_dict = { x:y for x,y in zip(names_list,coordinates_list)}

# Function to compute the distance between two points
def compute_city_distance_names(city_a, city_b, cities_dict):
    return compute_city_distance_coordinates(cities_dict[city_a], cities_dict[city_b])

def compute_city_distance_coordinates(a,b):
    return ((a[0]-b[0])**2+(a[1]-b[1])**2)**0.5
```

Based on the computed fitness, the progenitors are the lowest fitness values, because of their probabilities to mate and produce “descendants”. The algorithm selects a set of progenitors based on their mating probability. The selection process is executed as many times as necessary until we obtain enough progenitors to produce N kids to replace the original set of N solutions.

Genetics algorithm has different selection methods, such as Roulette wheel selection, rank selection, tournament selection etc. On this project, the roulette wheel is used for selecting potentially useful solutions for recombination, based on fitness proportionate. So, the function calculates a crossover individual probability, using individual's fitness divided by the sum of all population fitness.

$$p_i = \frac{f_i}{\sum_{j=1}^N f_j}$$

P_i (prob_list) is the probability of each chromosome equals the chromosome frequency divided by the sum of all fitness. Consequently, the probability of selecting a potential mate depends on your fitness with respect to the rest.

```
#define progenitor list
def progenitor_selection(population_set,fitness_list):
    total_fit = fitness_list.sum()
    prob_list = fitness_list/total_fit

    #notice there is the chance that a progenitor mates with oneself
    progenitor_list_a = np.random.choice(list(range(len(population_set))), len(population_set),p=prob_list, replace=True)
    progenitor_list_b = np.random.choice(list(range(len(population_set))), len(population_set),p=prob_list, replace=True)

    progenitor_list_a = population_set[progenitor_list_a]
    progenitor_list_b = population_set[progenitor_list_b]

    return np.array([progenitor_list_a,progenitor_list_b])
```

Two different progenitors list are generated and expected to mate. The mating consists of merging the two solutions into one (offspring) keeping bits of each of the parents (prog_a, prog_b). The (if not), checks if no repetitions exist in the offspring, otherwise, it will need to be corrected for the solution to satisfy the problem constraints.

```
#Crossover
def mate_progenitors(prog_a, prog_b):
    offspring = prog_a[0:5]

    for city in prog_b:

        if not city in offspring:
            offspring = np.concatenate((offspring,[city]))

    return offspring

def mate_population(progenitor_list):
    new_population_set = []
    for i in range(progenitor_list.shape[1]):
        prog_a, prog_b = progenitor_list[0][i], progenitor_list[1][i]
        offspring = mate_progenitors(prog_a, prog_b)
        new_population_set.append(offspring)

    return new_population_set
```

After the reproduction, a new population set, the algorithm has a mutate step, which is important to prevent local optima solutions. For this reason, randomness function will change different parts of the solution arbitrarily. Higher the variation of the progenitors, higher the chances of achieving a better solution, otherwise it can converge to all the solutions being the same. The *mutation_rate* parameter defines the percentage of progenitors that will be mutate for a new evaluation.

```

#Mutation
def mutate_offspring(offspring):
    for q in range(int(n_cities*mutation_rate)):
        a = np.random.randint(0,n_cities)
        b = np.random.randint(0,n_cities)

        offspring[a], offspring[b] = offspring[b], offspring[a]

    return offspring

def mutate_population(new_population_set):
    mutated_pop = []
    for offspring in new_population_set:
        mutated_pop.append(mutate_offspring(offspring))
    return mutated_pop

```

Stopping criteria's of genetic algorithm are:

- The algorithm performed all the maximum iterations established
- There is a solution that satisfies the minimum route, because was found a fitness equal or better than we expected
- Overused resources as money, time, and computation.
- The algorithm seems unable to find something better and the current solution satisfies the requirements.

The goal is merging all this criteria's to find the best stopping rule for the optimization route.

```

for i in range(num_inter):
    #Saving the best solution
    if fitnes_list.min() < best_solution[1]:
        best_solution[0] = i
        best_solution[1] = fitnes_list.min()
        best_solution[2] = np.array(mutated_pop)[fitnes_list.min() == fitnes_list]

    progenitor_list = progenitor_selection(population_set,fitnes_list)
    new_population_set = mate_population(progenitor_list)

    mutated_pop = mutate_population(new_population_set)

#Best Result
print(best_solution)

#Time
genetic_teste_time = time.time() - start_time
print("--- %s seconds ---" % (genetic_teste_time))

```

5.5 Algorithms Implemented

TSP has been studied for a long time. We decided to use some already published algorithms as a guide for our project. The authors and original websites are:

- HILL-CLIMBING: published by A Name Not Yet Taken AB at <https://www.annytab.com/> [15]
- SIMULATED ANNEALING: published by A Name Not Yet Taken AB at <https://www.annytab.com/> [16]

- TABU SEARCH: published by Bartłomiej Jamiołkowski *aka* MindBreaker20 at <https://github.com/MindBreaker20>^[17]
 - GENETIC ALGORITHMS: published by Roc Reguant at <https://medium.com/@rocreguant>^[18]

Although we researched existing codes, profound changes had to be made in order to answer our questions and meet the requirements of our work.

6 Experimental Results

6.1 Datasets

The datasets used in the code execution are shown below. The indicated distances are in kilometers. Unfortunately, it is not possible to make the 37×37 dataset more readable, however all the information shown below is available in the notebook (Jupyter).

	Porto	Braga	Aveiro	Viana do Castelo
Porto	0	54	75	7
Braga	56	0	126	6
Aveiro	73	125	0	14
Viana do Castelo	75	61	146	

Fig.6 – Test dataset 4 x 4

	Lisboa	Porto	Braga	Setubal	Coimbra	Evora	Aveiro	Leiria	Faro	ana do Caste	Beja	Braganca	Castelo	Guarda
Lisboa	0	312	364	49	205	133	255	145	277	385	176	484	224	319
Porto	315	0	54	349	118	405	75	181	549	76	448	205	258	200
Braga	367	56	0	400	170	456	126	233	601	61	500	217	309	252
Setubal	50	347	399	0	240	99	290	180	244	420	143	519	259	354
Coimbra	207	117	169	240	0	242	60	73	441	191	340	283	140	152
Evora	133	402	453	99	294	0	345	235	226	475	80	462	195	290
Aveiro	256	73	125	290	59	346	0	122	490	146	389	268	199	158
Leiria	147	181	233	181	74	237	124	0	381	254	281	353	165	222
Faro	278	548	599	245	440	226	490	381	0	621	146	720	460	554
Viana do Cas	387	75	61	420	190	476	146	253	621	0	520	271	329	271
Beja	177	446	498	143	338	79	389	279	147	519	0	539	273	368
Braganca	511	206	216	545	283	461	271	378	745	272	541	0	272	177
Castelo Bran	227	255	307	260	140	195	198	164	461	329	274	271	0	99
Guarda	321	199	251	355	154	289	160	259	555	273	369	177	100	0

Fig.7 – Portugal cities and distances dataset 14 x 14

Fig.8 – European cities and distances dataset 37 x 37

After executing the proposed algorithms, we performed the comparison between the optimal routes obtained and the respective execution times of each one.

6.2 Experimental Results

Below are the tables with the results obtained using 500, 1.000, 5.000 and 10.000 iterations for each algorithm, took on March 30th 2022. The values may be slightly different from those shown on the notebook as there are small changes with each run.

Best routes:

500 iterations				1.000 iterations			
Example	Europe	Portugal	Teste	Example	Europe	Portugal	Teste
Algorithm				Algorithm			
Genetic	34943.000000	2403.000000	334.000000	Genetic	35131.000000	2334.000000	338.000000
Hill-Climbing	20554.000000	1996.000000	334.000000	Hill-Climbing	20554.000000	2160.000000	334.000000
Simulated Annealing	21148.000000	2684.000000	334.000000	Simulated Annealing	21532.000000	2710.000000	336.000000
Tabu Search	22193.000000	1814.000000	334.000000	Tabu Search	21067.000000	1928.000000	334.000000

5.000 iterations				10.000 iterations			
Example	Europe	Portugal	Teste	Example	Europe	Portugal	Teste
Algorithm				Algorithm			
Genetic	35433.000000	2408.000000	338.000000	Genetic	31715.000000	2715.000000	338.000000
Hill-Climbing	21209.000000	2160.000000	334.000000	Hill-Climbing	21433.000000	1853.000000	334.000000
Simulated Annealing	22903.000000	2146.000000	334.000000	Simulated Annealing	21983.000000	2219.000000	334.000000
Tabu Search	19583.000000	2149.000000	334.000000	Tabu Search	17339.000000	1695.000000	334.000000

Fig.9 – Best route in Km. In all runs (~30x). Best results highlighted in green.

Best run times:

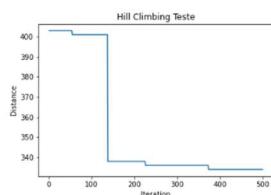
500 iterations				1.000 iterations			
Example	Europe	Portugal	Teste	Example	Europe	Portugal	Teste
Algorithm				Algorithm			
Genetic	2.061837	0.823812	0.254758	Genetic	4.460856	1.727222	0.529009
Hill-Climbing	0.056075	0.026979	0.007990	Hill-Climbing	0.104893	0.033966	0.021976
Simulated Annealing	0.050189	0.020968	0.085912	Simulated Annealing	0.103894	0.123472	0.043954
Tabu Search	0.050417	0.067387	0.005980	Tabu Search	0.075913	0.062918	0.009981
5.000 iterations				10.000 iterations			
Example	Europe	Portugal	Teste	Example	Europe	Portugal	Teste
Algorithm				Algorithm			
Genetic	21.023144	7.705487	2.349869	Genetic	43.742670	15.833771	4.824254
Hill-Climbing	0.447905	0.215780	0.134584	Hill-Climbing	0.969232	0.664925	0.397601
Simulated Annealing	0.435094	0.255421	0.245766	Simulated Annealing	0.986990	0.660251	0.513638
Tabu Search	0.218802	0.102895	0.046951	Tabu Search	0.277762	0.161844	0.091907

Fig.10 – Time of execution in seconds. In all runs (~30x). Best results highlighted in green.

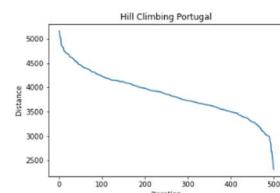
6.3 Iterations x Route Graphs (plus Temperature for Sim. Annealing only)

Hill Climbing

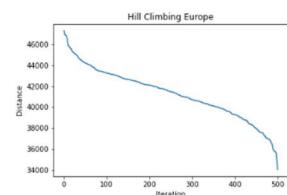
4 x 4 – 500 iterations



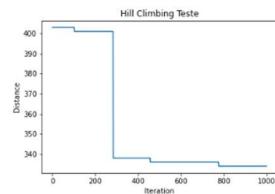
14 x 14 – 500 iterations



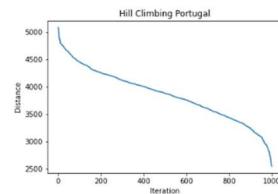
37 x 37 – 500 iterations



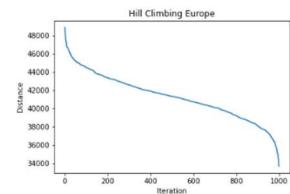
4 x 4 – 1.000 iterations

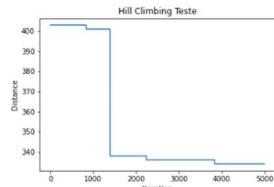
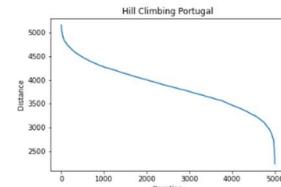
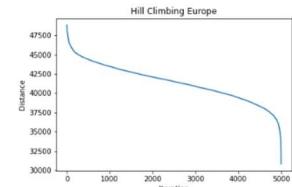
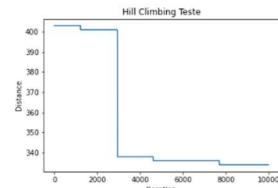
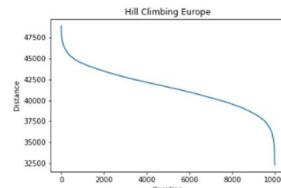
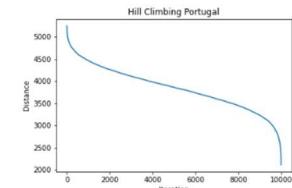


14 x 14 – 1.000 iterations

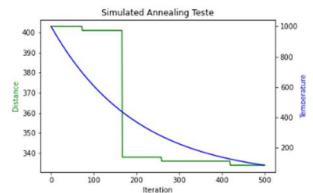
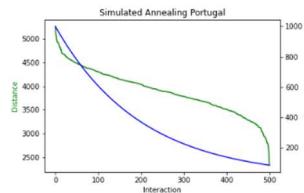
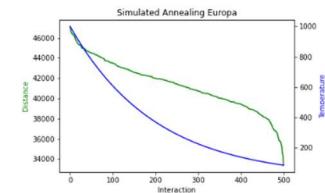
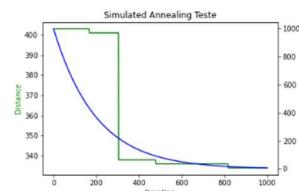
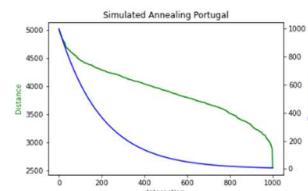
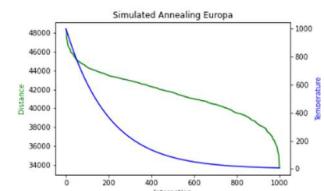
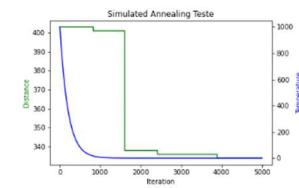
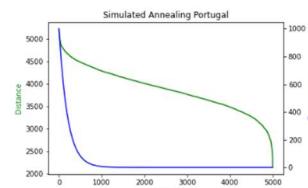
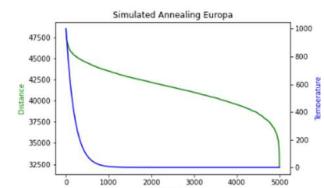


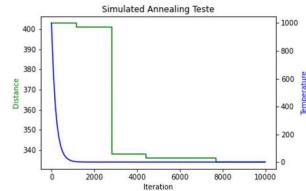
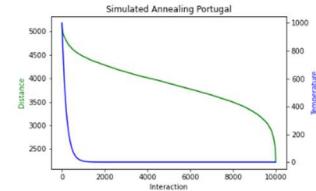
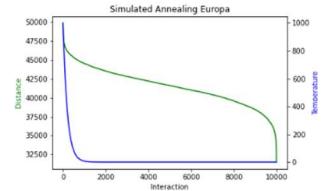
37 x 37 – 1.000 iterations



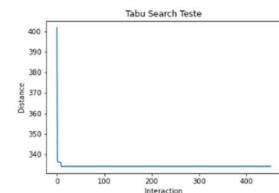
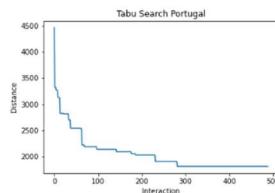
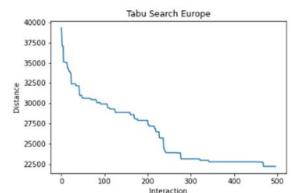
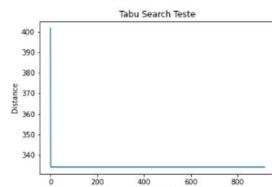
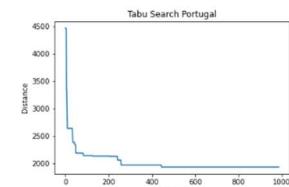
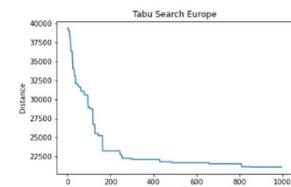
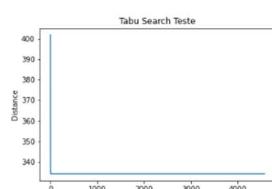
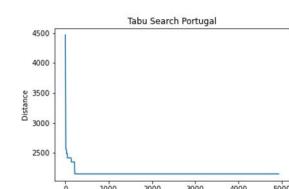
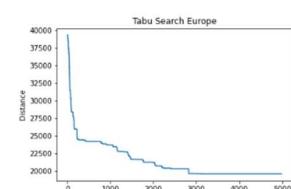
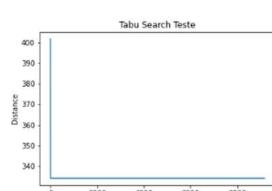
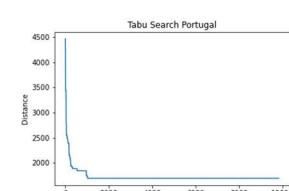
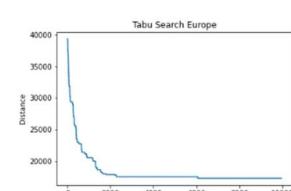
4 x 4 – 5.000 iterations**14 x 14 – 5.000 iterations****37 x 37 – 5.000 iterations****4 x 4 – 10.000 iterations****14 x 14 – 10.000 iterations****37 x 37 – 10.000 iterations**

Simulated Annealing

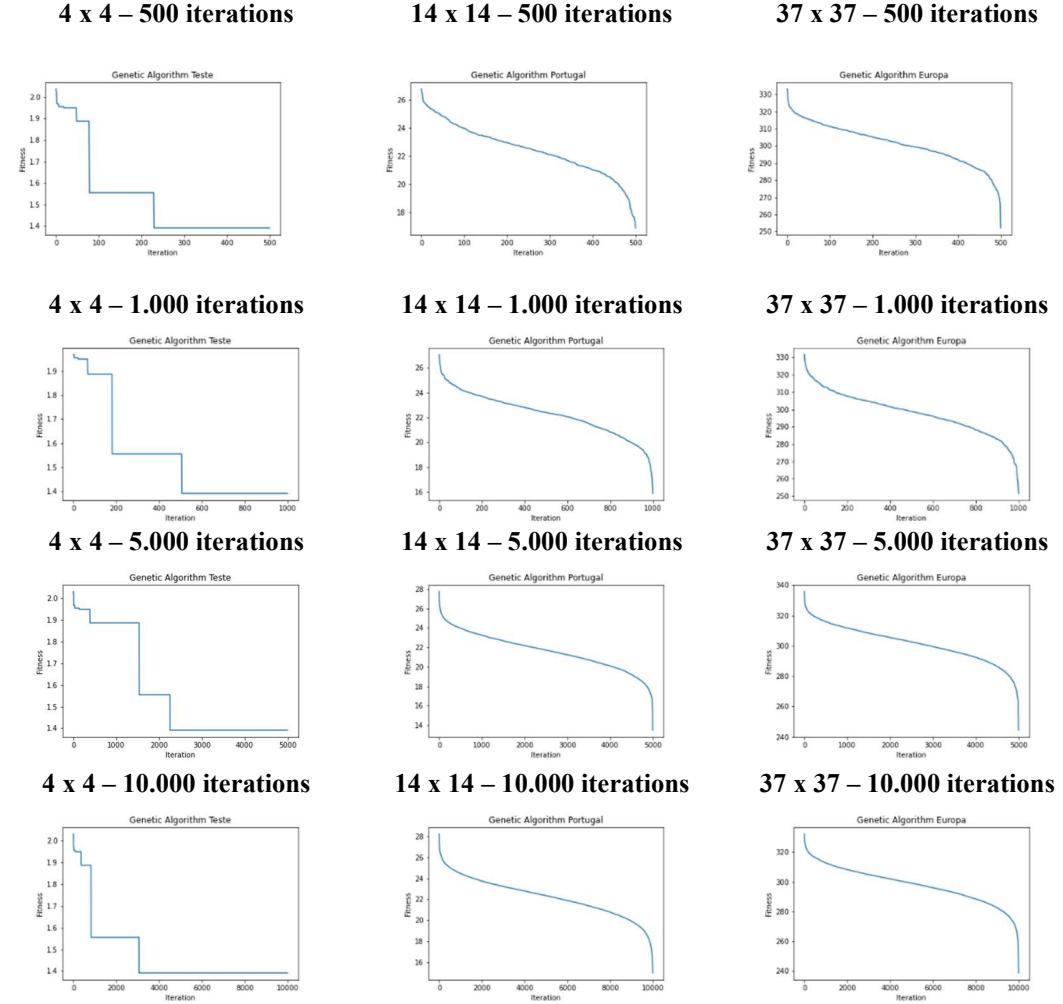
4 x 4 – 500 iterations**14 x 14 – 500 iterations****37 x 37 – 500 iterations****4 x 4 – 1.000 iterations****14 x 14 – 1.000 iterations****37 x 37 – 1.000 iterations****4 x 4 – 5.000 iterations****14 x 14 – 5.000 iterations****37 x 37 – 5.000 iterations**

4 x 4 – 10.000 iterations**14 x 14 – 10.000 iterations****37 x 37 – 10.000 iterations**

Tabu Search

4 x 4 – 500 iterations**14 x 14 – 500 iterations****37 x 37 – 500 iterations****4 x 4 – 1.000 iterations****14 x 14 – 1.000 iterations****37 x 37 – 1.000 iterations****4 x 4 – 5.000 iterations****14 x 14 – 5.000 iterations****37 x 37 – 5.000 iterations****4 x 4 – 10.000 iterations****14 x 14 – 10.000 iterations****37 x 37 – 10.000 iterations**

Genetic Algorithm



6.4 Illustrative Route Maps

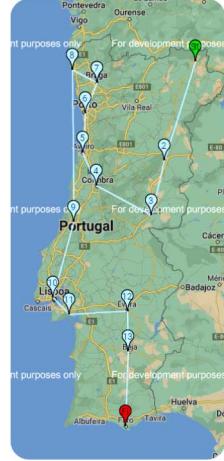
These routes maps were obtained as a result of each simulation with best results collected at Fig. 9. We can see the many differences in the "interpretation" of each algorithm to draw the route.

HC 4 x 4 1000 it

334 Km

**HC 14 x 14 1000 it**

2160 Km

**Hill Climbing 37 x 37 1000 it**

20554 Km

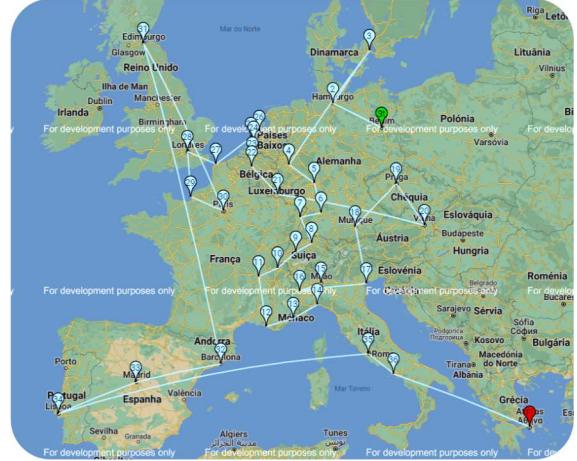


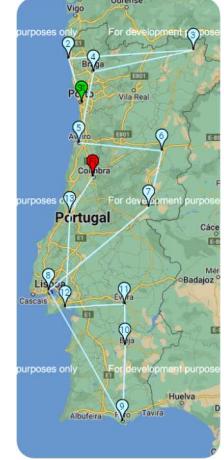
Fig.11 – Hill-Climbing route map after 1.000 iteration

SA 4 x 4 5000 it

334 Km

**SA 14 x 14 50000 it**

2146 Km

**Simulated Annealing 37 x 37 5000 it**

22903 Km

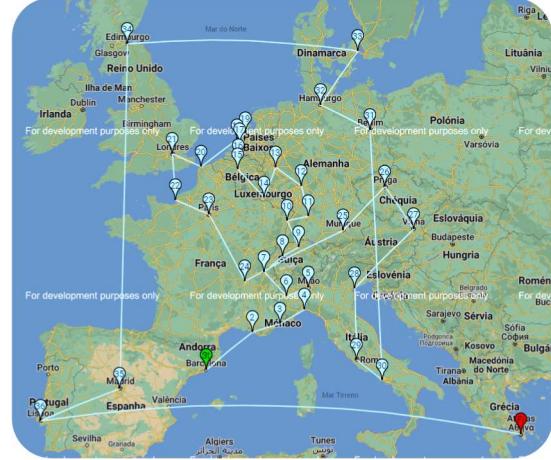


Fig.12 – Simulated Annealing route map after 5.000 iterations

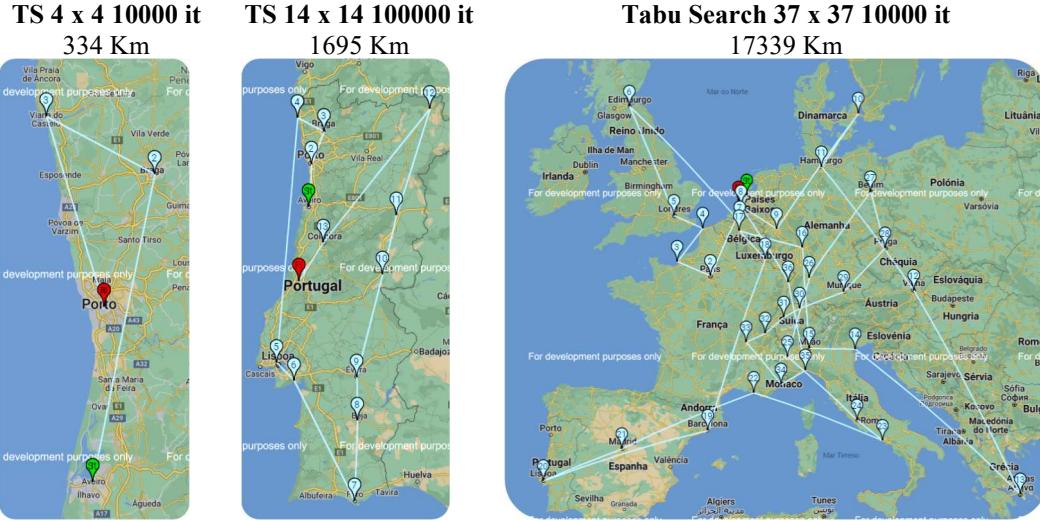


Fig.13 – Tabu Search route map after 10.000 iterations

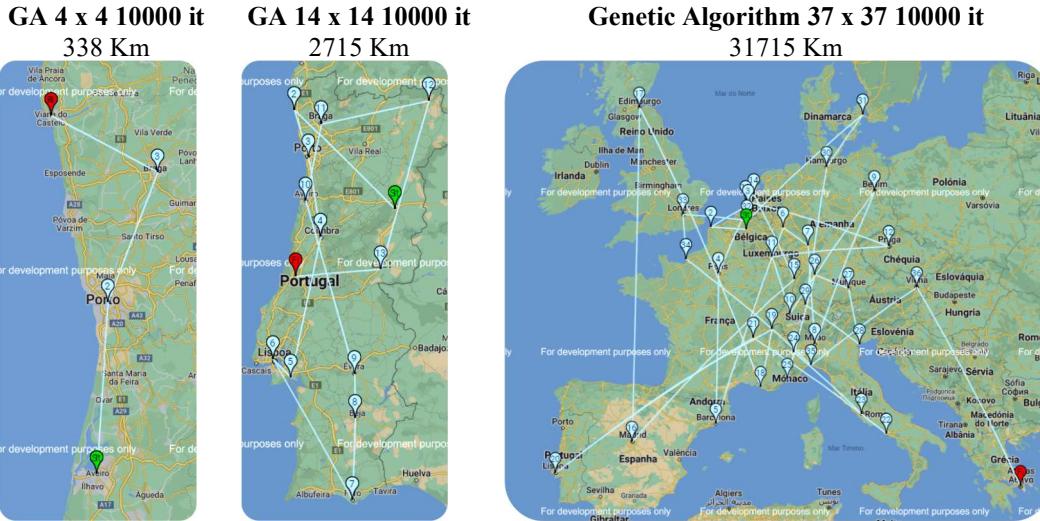


Fig.14 – Genetic Algorithm route map after 10.000 iterations

7 Conclusion

The results were obtained with the following algorithms parameters specification:

- Hill Climbing:
 - Iterations: 500, 1.000, 5.000 and 10.000.
 - Neighborhood: random swap among two neighbors.
 - Mutation rate: mutation_rate = 0.7 (discarding 30% neighbourhood).

- Simulated Annealing:
 - Iterations: 500, 1.000, 5.000 and 10.000.
 - Neighborhood: random swap among two neighbors.
 - Temperature: Initial 1000°, final 0°.
 - Mutation rate: mutation_rate = 0.7 (discarding 30% neighbourhood).
- Tabu Search:
 - Iterations: 500, 1.000, 5.000 and 10.000.
 - Tabu tenure:
 - Tabu len test = 2 iterations
 - Tabu len Portugal = 4 iterations
 - Tabu len Europe = 6 iterations
 - Neighborhood: set 1 for test, Portugal, and Europe.
- Genetic Algorithm:
 - Iterations: 500, 1.000, 5.000 and 10.000
 - n_cities: length of cities in each matrix (4, 14 and 37)
 - n_population: 50. number of populations that will be generated in genesis function by the initial progenitor
 - mutation_rate: 0.3. percentage of progenitors that will be mutate for a new evaluation.

As shown in Fig. 9 – Page 22, the all the algorithms presented the best results (334 Km) with 500 iterations to the test dataset. We also can see that:

- The best route for Portugal cities were found for Tabu Search with 10.000 iterations (1.695 Km). It's 6,5 % better than the best result with 500 iterations and to get this 6,5% improvement, we need to use 140% more time
- The best route for Europe cities were also found for Tabu Search with 10.000 iterations (17.339 Km). It's 15,6% better than the best result with 500 iterations and to get this 15,6% improvement, we need to use 395% more time.

Portugal			Europe		
Route (Km)	Time (s)	Alg.	Route (Km)	Time (s)	Alg.
FBR 500 it	1814	0,067387	Tabu S.	20554	0,056075
BR 10.000 it	1695	0,161844	Tabu S.	17339	0,277762
Variation	-6,56%	140,17%		-15,64%	395,34%

FBR = First Best Route, BR = Best Route

It is clear that these times are very small, less than 1 second, however, for future work with larger universes of cities or locations, the impact of this increase in processing time must be evaluated. Complete time processing at Fig. 10 – Page 23.

The Fig. 9 and 10 show the cost-benefit ratio of increasing the number of iterations with fixed algorithm parameters to get their best solution route. Most of the algorithms performed their best local solution in less than one second, except for the genetic, which

was much slower. Therefore, as most of the output processing time were fast, the individual parameters of each algorithm were analyzed and modified with the aim of searching for new possible better routes with less time in the European dataset and 10.000 iterations.

- Hill Climbing:
 - Iterations: 10.000.
 - Neighborhood: random swap among two neighbors.
 - Mutation rate: mutation_rate = 1 (no discarding neighb.).
- Simulated Annealing:
 - Iterations: 10.000.
 - Neighborhood: random swap among two neighbors.
 - Temperature: Initial 1000°, final 1°.
 - Mutation rate: mutation_rate = 1 (no discarding neighb.).
- Tabu Search:
 - Iterations: 10.000.
 - Tabu tenure:
 - Tabu len Europe = 2 iterations (keeping Tabu for 2 it.).
 - Neighborhood: 2 (generate neighbors two times swapping cities).
- Genetic Algorithm:
 - Iterations: 10.000.
 - n_cities: 37.
 - n_population: 100. Number of populations that will be generated in genesis function by the initial progenitor.
 - mutation_rate: 0.4. Percentage of progenitors that will be mutate for a new evaluation, avoiding local maxima.

There was no improvement in the results already obtained, as can be seen in the figure below:

Example	Europe
Algorithm	
Genetic	32668.000000
Hill-Climbing	21615.000000
Simulated Annealing	22132.000000
Tabu Search	19175.000000

Example	Europe
Algorithm	
Genetic	828.686554
Hill-Climbing	1.720625
Simulated Annealing	0.216883
Tabu Search	0.725888

Fig.15 – Route and time processing for Europe dataset, modifying parameters.

Finally, we performed a complete round with 1,000,000 iterations, keeping the parameters of the initial test (pages 28-29). Still, we didn't get better results.

Example	Europe	Portugal	Teste
Algorithm			
Genetic	33459.000000	2168.000000	338.000000
Hill-Climbing	21085.000000	1695.000000	334.000000
Simulated Annealing	22712.000000	1916.000000	334.000000
Tabu Search	19518.000000	1700.000000	334.000000

Example	Europe	Portugal	Teste
Algorithm			
Genetic	9038.901190	6849.501923	5361.153966
Hill-Climbing	8547.086568	8494.370667	8472.803038
Simulated Annealing	104.815753	102.602015	96.971790
Tabu Search	23.853625	12.248454	7.291541

Fig.16 – Route and time processing for all datasets, 1M iterations.

So, we concluded our work verifying that the best results were found using Tabu Search, with 10,000 interactions and with the following parameters:

- Tabu tenure:
 - Tabu len test = 2 iterations
 - Tabu len Portugal = 4 iterations
 - Tabu len Europe = 6 iterations
- Neighborhood: set 1 for test, Portugal, and Europe.

Example	Europe	Portugal	Teste
Algorithm			
Tabu Search	17339.000000	1695.000000	334.000000

Fig.17 – Best results. Run Time: 0.27s, 0.16s and 0.09s respectively.

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