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Nature-inspired Monte Carlo optimization

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Abstract

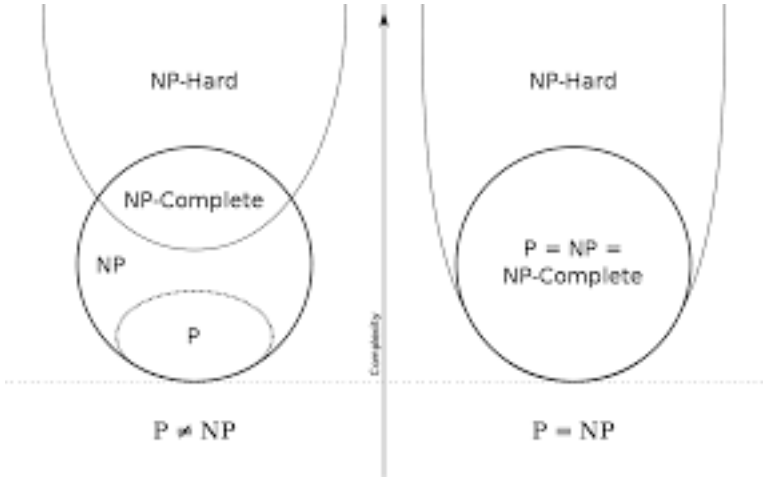
The aim of this project is to solve the travelling salesman problem (TSP) which consists in finding the shortest hamiltonian cycle among all the cities.
The problem is a *NP-hard* problem and therefore there exist no feasible algorithm to solve exactly for any possible set of cities in input. The appromximatively optimal solution was computed by the simulated annealing, while the possible cycles are produced by a genetic algorithm.
The report shows the result of the simulations computed on some cities of northern italy and compares the exact feasible solutions with the approximated ones.

1 Introduction

The travelling salesman problem (TSP) consists in finding the shortest route a travelling salesman has to take to visit all the city only once and to return to the starting point. The route described is called *hamiltonian cycle* in graph theory (i.e. a cycle that pass through each vertex of a graph just once), indeed the oldest and more technical formulation of the problem was proposed by Hamilton. An algorithm that provides a solution to the travelling salesman problem can be exploited in a wide variety of applications: indeed it can be used in logistics to optimize the path of vehicles and therefore to reduce costs. It is possible to model the problem usign an undirected, weighted and fully connected graph [1] $G = (N, E)$, where N is the set of the cities to visit and $E = N \times N$ is the weight of the path. In this particular instance of the problem the weights correspond to the euclidean distance between each couple of cities. Formally, an hamiltonian cycle can be defined as a sequence $(n_0, .., n_{k-1})$ of length k such that $n_i \neq n_j \ \forall i, j \in \{1, ..., |N|\}$.

1.1 Hardness of the travelling salesman problem

Solving the travelling salesman problem pose very tricky computational problems. Indeed, the most intuitive solution to the problem consist in computing all the possible paths and then evaluate all their lengths to find the shortest. But the number of possible cycles is $(n-1)!$ and grows faster that 2^n (i.e. $2^n = o(n!)$) and thus the problem cannot be solved in finite time for large n. Morover, even if it was possible to generate each hamiltonian cycle in constant time independently from their length, the algorithm will have an exponential time complexity to find the best result.
More techically, TSP is an *NP-hard* problem, meaning that it is at least as hard as the hardest NP-complete problem. *NP-complete* problems are problems that can be solved in polynomial time by a non-deterministic algorithm. For such a class of problem there exists no polynomial algorithm that can solve the problems and may not exist, still noone was able to prove that such algorithms does not exists.



[1] For an hamiltinian cycle to exist the graph must be at least connected

Bearing in mind the complexity problem to face, the most reasonable solution is to solve the problem approximatively. The technique I used to generate the possible hamiltonian cycles is a genetic algorithm, while the choice of the shortest hamiltonian cycle is done by the *simulated annealing* algorithm.

2 Simulated annealing

Simulated annealing (SA) is a technique that mimic the behaviour of heated materials slowly cooled down in metallurgy, this process decreases the impurity and increases the size of the crystals meaning that allows materials to reach the state that minimizes the energy. It is a technique to approximate the global optimal solution when the solutions is to be searched in an enormous space. SA is a metaheuristic meaning that it is not a probelm-specific stochastic heuristic. As every metaheuristic algorithm it relies on two principles *intensitification* and *diversification*, indeed, the algorithm intensifies the search near different possible optimal solutions. SA is very useful since it does not require any prior information, other than the cost, indeed it just supposes that states (hamiltonian cycles in our case) are distributed accordingly to the Bolzmann distribution:

$$e^{-\beta(cost(state))} \tag{1}$$

The Boltzmann distribution is suitable to model the TSP problem since it is most unbiased distribution among all the possible distributions. The undiasedness derives from the maximization of the Shannon entropy, given the cost. [METTI UNA CITAZIONE]
The underlying assumption of simulated annealing is that the optimal states are the states with the lowest cost, and they are reached as the temperature decreases. The temperature T is the inverse of β ($T = \frac{1}{\beta}$), therefore we start with low values of β (high temperature) and as the simulation proceeds we increase the values of β, thus mimicking the decrease in temperature. The only other information needed is the cost function. For this specific application the cost function is the sum of euclidean distances between the cities in the cycle. The coordinate of a city (x, y) are expressed in longitude and latitude.
In the following we provide a schematic overview of the simulated annealing implemented.

```
1: function SIMULATED ANNEALING(betas,number of simulations)
2:     s ← generate starting state with the genetic algorithm
3:     for b in betas do
4:         for n in 1,.., number of simulations do
5:             ns ← generate a new state with the genetic algorithm starting from s
6:             ns ← METROPOLIS(s,ns,β)
7:         end for
8:     end for
9:     return ns
10: end function
```

where **betas** is a set of the values of β.
The code executes all the procedures using a vectorial implementation to speed up the computation.

3 Metropolis algorithm

Metropolis is a Markov Chain Monte Carlo (MCMC) algorithm used to generate values X_n from a finite set of values S accordingly to a target probability distribution π.
An homogeneous and finite Markov chain with state space S, transition matrix P and initial distribution μ is a sequence of random variables $\{X_n\}_{n\in N}$ such that

1. $\forall i \in S\, Pr(X_0 = i) = \mu(i)$
2. $\forall n > 0\ \forall i_n, ..., i_0\, Pr(X_{n+1} = j | X_n = i_n, ..., X_0 = i_0) = Pr(X_{n+1} = j | X_n = i)$
3. $\forall n > 0\, Pr(X_{n+1} = j | X_n = i) = p(i, j)$

Metropolis algorithm is designed in such a way that it is very likely to move from a state with lower probability from a state with higher probability.
The following algorithm describes the metropolis algorithm when the target distribution is $\pi(\text{state}) = e^{-\beta\, \text{cost(state)}}$ and S is the set of all possible hamiltonian cycles having fixed their length. In the following we suppose to have generated two hamiltonian cycles (i.e states) old_state, new_state and we want to understand if new_state can come from π. If new_state is likely to be a sample of π we use it as new state otherwise we keep old_state as the current state.

```
1: function METROPOLIS(old_state, new_state, β)
2:     if cost(new_state) < cost(new_state) then
3:         return new_state
4:     end if
5:     threshold ← unif[0,1]
6:     p ← min{1, e^{−β(cost(new_state)−cost(old_state))}}
7:     if p > threshold then
8:         return new_state
9:     else
10:        return old_state
11:    end if
12: end function
```

3.1 Properties of metropolis algorithm

We can model the generation of new hamiltonian cycles using a undirected and connected graph $G = (S, E)$ whose set of states S contains all the possible hamiltonian cycles and E contains the transition probability from an hamiltonian cycle to another one. Given the graph, we can define the transition matrix $P = p(i, j)]_{i,j\in S}$ as

$$p(i,j) = \begin{cases} 0 & \text{if } \{i,j\} \notin E \\ \frac{1}{d_i} \min\{1, \frac{\pi(j)}{\pi(i)}\} & \text{if } \{i,j\} \in E\ ,\ i \neq j \\ 1 - \frac{1}{d_i} \sum_{l \in adj(i)} \min\{1, \frac{\pi(l)}{\pi(i)}\} & \text{if } i = j \end{cases} \tag{2}$$

Since G is a connected graph, the P is irriducible meaning that $\forall i, j \in S\, p^n(i, j) > 0$, where $p^n(i, j)$ means that exist a path from i to j of length n.

It can also be proved that P is aperiodic [1]. By aperidoicity we mean each node of the graph has a loop. More formally, th graph G is aperiodic if $\forall i \in S$, $d(i) = 1$ where

$$d(i) = mcd\{n \in N | \text{ exist a cycle from i to i of length } n\} \tag{3}$$

Metropolis algorithm defines a probability distributin π that is a reversible distribution, meaning that

$$\pi(i)p(i,j) = \pi(j)p(j,i) \;\; \forall i,j \in S \tag{4}$$

This is a key feature of the algorithm since a reversible distribution π is also a stationary distribution $\pi' P = \pi'$. This condition holds by the following theorem

Theorem 1. *If a probability distribution π is a reversible distribution for a markov chain $\{X_n\}$, then it is also a stationary distribution.*

Proof. $(\pi' P)_j = \sum_{i \in S} \pi(i)p(i,j) = \sum_{i \in S} \pi(j)p(j,i) = \pi(j)$ □

If this distribution was unique than we are certain to correctly generate the data accordingly to the target distribution. The stationary distibution is unique if the transition matrix is primitive as stated by the follwing theorem.

Theorem 2. *Let $\{X_n\}$ be a markov chain with a primitive (i.e. irreducible and aperiodic) transition matrix on a finite set, then there exist only one stationary distribution and it as also the limit distribution* $\lim_{n \to \infty} p^n(i,j) = \pi(j) \, \forall i \in S$

Since P is primitive, it is enough to compute the limit distribution to find the unique stationary distribution.
The stationary distribution can be approximated in a logarithmic number of iterations starting from any distribution. Therefore to sample hamiltonian cycle from the stationary distribution is enough to let the simulation go on for a suitable number of iterations.
METTI CITAZIONE LIBRO

4 Genetic Algotirthm

Genetic algorithms are a widespread clarclengthss of algorithms that mimic nature. Indeed there are three fundamental operations they perform to generate new states (hamiltonian cycles in our case), each operation is inspired by the theory of evolution by C. Darwin.
Among a specie, evolution selects the fittest individuals and therefore the algorithm will chose the fittest (i.e shortest) hamiltonian cycles.
The breeding of the fittest individuals produces new individuals that inherits traits from the parents, therefore in the crossbreeding phase we mix some subsection of the fittest hamiltonian cycles.
As random mutations can occur in nature but they are not so likely to occur, the algorithms swaps two cities with a fixed and low probability. The mutation probability should be low since otherwise if can disrupt the optimal subsequence of the cycle inherited.
My own implementation of the algorithms performs the selection operation as follows:

```
function SELECTION(population,n_paths)
    n_parents ← unif[2,n_paths/2]
    order the population by fitness
    fittest_subpopulation ← extract n_parents in order from the sorted population
    return fittest_subpopulation
end function
```

where **population** is an array of hamiltonian cycles.

```
function CROSSBREEDING(fittest_subpopulation)
    for i in 1, ..., n_paths do
        choose parent1 uniformely among the fittest_subpopulation
        Choose parent2 uniformely among the fittest_subpopulation
        if parent1 different from parent2 then
            choose position1 randomly among unif([0,length of cycles-1)
            choose position2 randomly among unif([0,length of cycles-1)
            divide parent1 in three sections:
            [parent10:position1]
            parent1[position1:position2]
            parent1[posotion2:]
            divide parent2 in three sections:
            parent2[0:position1]
            parent2[position1:position2]
            parent2[posotion2:]
            breed child1 justapposing in the order:
            parent1[0:position1]
            all the cities not in parent1[0:position1] and not in parent2[posotion2:]
            parent2[posotion2:]
            breed child2 justapposing in the order:
            parent2[0:position1]
            all the cities not in parent2[0:position1] and not in parent1[posotion2:]
            parent1[posotion2:]
        else
            child1 ← parent1
            child2 ← parent1
        end if
    end for
    new_population is a vector of the children
end function
```

```
1: function MUTATE(new_population, p)
2:     for path in new_population do
3:         test ← unif[0,1]
4:         if test < p then
5:             choose position1 randomly among unif[0,length of cycles-1)
6:             choose position2 randomly among unif[0,length of cycles-1)
7:             swap the cities in position1 and position2
8:         end if
9:     end for
10:    return new_population
11: end function
```

```
1: function EVOLVE(population)
2:     fittest_population ← SELECT(population)
3:     new_population ← CROSSBREED(fittest_population)
4:     population ← MUTATE(new_population)
5: end function
```

5 dataset

6 results

References

[1] Oliver Catoni *Simulated annealing algorithms and Markov chains with rare transitions*, Sminaire de probabilits (Strasbourg), tome 33 (1999), p. 69-119.