INFO-H-413 - Learning Dynamics: Implementation Exercise #2 The Traveling Salesman Problem with Time Windows - Stochastic Local Search Algorithms

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Implementation

The heuristic solver had been written using the C++ programming language, in order to be able to take adventage of the functionalities offered by the Standard Template Library (STL).

By combining an object-oriented approach with those functionalities, I built a modular application core (Heuristic Core) that has been used for the two exercises required for this implementation.

The core is directly linked with the reader (*InstanceReader*) which reads the files containing all the informations to run the simulation (distance matrix, time windows vector and seeds list) and the writer (*Writer*) which outputs the results of the simulation in a CSV file.

Two different command line front-ends, sharing the same underlying structure, but having a different set of parameters, have been developed to distinguish the iterative-improvement interface from the variable neighborhood descent one.

The global program structure is depicted here:

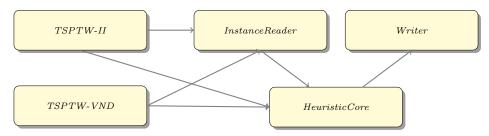


Figure 1: Simulation Code Structure

The names of the nodes corresponds to those of the implementation (.cpp) and header files for the corresponding classes. In addition to these, a class to represent the time windows (TimeWindow.h) and another one to represent the candidate solution as a user defined data type (CandidateSolution.{h,cpp}) have been implemented.

How to compile the program?

The software was developed in C++98 under Linux (Debian Wheezy), using the GNU g++ (Debian 4.7.2-5) 4.7.2 compiler and tested in this environment. The software is distributed as a compressed tar file, containing both the source code (in the src folder) and the scripts and instances (in the bin and bin\instances respectively). To install the program, first obtain the file TSPTW.V1.0.tar.gz. Unzip the file by typing:

gunzip TSPTW.V1.0.tar.gz

and then unpack it by typing:

tar -xvf TSPTW.V1.0.tar

The software will be extracted in a new folder TSPTW.V1.0 Finally, by launching

make all

the Makefile will trigger the compilation of the files, producing the executables 'TSPTW-II' and 'TSPTW-VND" in the bin folder.

Note: The code is written in C++98. Hence, the code should be reasonable portable to other Operating Systems than Linux or Unix.

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How to run the program?

Once the program has been compiled, two separate executable files, corresponding to the different kind of metaheuristic (i.e. Iterative Improvement and Variable Neighborhood Descent) can be either launched directly via the command line interface or using the bash script to launch.

The design choice to separate the two different kind of metaheuristic is made in order to limit the number of command line parameters to be given as input to the program.

Command-line execution

By launching¹:

```
./TSPTW-II [PARAMETERS] -i [INPUT_FILE] -s [SEEDS_FILE]
./TSPTW-VND [PARAMETERS] -i [INPUT FILE] -s [SEEDS FILE]
```

one can display the information about the meaning of the different options that can be given as input to the program.

Additional information concerning the usage of the program can be found in the README file.

The only mandatory options are "-i, -input" and "-s,-seeds", since without these components will not be possible to execute the simulation.

The argument to the input option must contain the full path to the instance file.

The seeds file must contain a number of seeds at least equal to the number of runs required, one seed per line without any additional information.

The options controlling the same parameters are mutually exclusive, with that meaning that only one option must be selected in order to run the program. If multiple options for the same parameter are chosen, the program will not run.

TSPTW-II

Parameter	Mutually exclusive options
Initial solution	-d,-random , -h,-heuristic
Neighborhood type	-t,-transpose , -e,-exchange , -n,-insert
Pivoting rule	-f,-first-imp , -b,-best-imp

TSPTW-VND

Parameter	Mutually exclusive options
VND algorithm	-t, -standard, -p, -piped
Neighborhood chain	-a,-TEI , -b,-TIE

Output Every experiment produces a single file:

- (II) [$pivoting_rule$].[$neighborhood_type$].[$INSTANCE_NAME$] with [$pivoting_rule$] $\in \{first, best\}$ and [$neighborhood_type$] $\in \{transpose, exchange, insert\}$
- (VND) $[vnd_type]$. $[neighborhood_chain]$. $[INSTANCE_NAME]$ with $[vnd_type] \in \{standard, piped\}$ and $[neighborhood_type] \in \{tei, tie\}$

Examples:

```
exchange.best.n80w200.004.txt standard.tei.n80w20.003.txt
```

The internal structure of the file is the following: Seed CV CpuTime PRPD

For each run of the algorithm, the program writes in the file, using a tabulation as separator, the used seed, the number of constraints violations, the cpu runtime and the penalised relative percentage deviation.

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¹The squared-bracket notation implies that the formal parameters to the script have to be substituted by their actual value.

Script execution

By launching:

- ./launchTSPTW-II.sh [INSTANCE NAME] [RUNS] [SEEDS FILE]
- ./launchTSPTW-VND.sh [INSTANCE NAME] [RUNS] [SEEDS FILE]

The script will:

- 1. Create the files required by the data processing script to write statistics.
- 2. Generate a seed file, named [SEEDS_FILE] containing [RUNS] randomly generated seeds.
- 3. Launch the corresponding TSPTW program for [RUNS] using all the possible combinations of input options.
- 4. Wait for the termination of all the previously launched experiment and call the R data processing script

The script assumes that all the instances are located into the instances folder, hence it is only necessary to indicate the instance name, instead of the complete path.

Output Each execution of the script will then generate the files:

- [INSTANCE_NAME] CpuTime.pdf containing the boxplots of the runtime distribution for each algorithm.
- [INSTANCE_NAME] PRPD.pdf containing the boxplots of the PRPD distribution for each algorithm.
- (II) transpose.first, exchange.first, insert.first, transpose.best, exchange.best, insert.best
 - (VND) standard.tei, standard.tie, piped.tei, piped.tie

The internal structure of the file is the following:

Instance Infeasible mean(PRDP) mean(CpuTime)

Each line contains the instance name, the percentage of infeasible runs, the mean PRDP and the mean runtime across [RUNS] runs.

Problem formulation

An instance of the Travelling Salesman Problem with Time Windows (TSPTW) can be expressed as a tuple $\langle N, E, c, t \rangle$ where:

- $N: \{0, \cdots, n\}$ Node set
- $E: N \times N$ Edge set
- $c: E \mapsto \mathbb{R}$ Edge cost function mapping a cost c to every edge $e \in E$.
- $t: N \mapsto \mathbb{R}^2$ Time window function mapping a couple of values a_i, b_i representing respectively, the opening and closing time of the time window, such that $a_i < b_i$, to every node $i \in N$.
- A candidate solution for the problem, in this case, is represented as a permutation p of the nodes in N, where p_i represents the i^{th} solution component (node) in the sequence, such that $p_0 = 0 \forall p$.

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As in [6] the formal definition of the problem is:

$$\mathbf{min} \quad f(p) = \sum_{i=0}^{n} c(e_{p_i p_{k+i}})$$

$$\mathbf{subject to} \quad \Omega(p) = \sum_{i=0}^{n+1} \omega(p_i) = 0$$
(1)

where

$$\omega(p_i) \begin{cases} 1 & A_{p_i} < b_{p_i} \\ 0 & \text{otherwise} \end{cases}$$

$$A_{p_{i+1}} = \max(A_{p_i}, a_i) + c(e_{p_i p_{k+i}})$$

$$(2)$$

As one may notice in 1 and 2, a feasible solution p for the problem is a permutation where the constraints related to the time windows are met for every node i in the permutation.

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Problem 1

Ant Colony Optimization

Problem statement

Implement two stochastic local search (SLS) algorithms for the traveling salesman problem with time windows (TPSTW), building on top of the perturbative local search methods from the first implementation exercise.

- 1. Run each algorithm 25 times with different random seed on each instance. Instances will be available from http://iridia.ulb.ac.be/~stuetzle/Teaching/HO/. As termination criterion, for each instance, use the maximum computation time it takes to run a full VND (implemented in the previous exercise) on the same instance and then multiply this time by 1000 (to allow for long enough runs of the SLS algorithms).
- 2. Compute the following statistics for each of the two SLS algorithms and each instance:
 - Percentage of runs with constraint violations
 - Mean penalised relative percentage deviation
- 3. Produce boxplots of penalised relative percentage deviation.
- 4. Determine, using statistical tests (in this case, the Wilcoxon test), whether there is a statistically significant difference between the quality of the solutions generated by the two algorithms.
- 5. Measure, for each of the implemented algorithms on 5 instances, the run-time distributions to reach sufficiently high quality solutions (e.g. best-known solutions available at http://iridia.ulb.ac.be/~manuel/tsptw-instances#instances). Measure the run-time distributions across 25 repetitions using a cut-off time of 10 times the termination criterion above.
- 6. Produce a written report on the implementation exercise:
 - Please make sure that each implemented SLS algorithm is appropriately described and that the computational results are carefully interpreted. Justify also the choice of the parameter settings and the choice of the iterative improvement algorithm for the hybrid SLS algorithm.
 - Present the results as in the previous implementation exercise (tables, boxplots, statistical tests).
 - Present graphically the results of the analysis of the run-time distributions.
 - Interpret appropriately the results and make conclusions on the relative performance of the algorithms across all the benchmark instances studied.

Introduction

Ant Colony Optimization is an example of population-based metaheuristic (i.e a set of algorithmic concepts that can be used to define heuristic methods) inspired by the behavior of the ant species *Iridomyrmex humilis*. To be more precise, these insects are able, by means of stigmergic communication, to choose the shortest path between their nest and a food source, when given the choice ([2]).

The communication process occurs by deposing a certain quantity of pheromone in the environment that can be sensed by the other ants and that will be used by them as an heuristic (i.e an information to guide their choice) for selecting the shortest path.

Furthermore, the pheromone quantity on a certain location decreases over time because of evaporation, thus requiring a continuous deposit process to be effective.

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The convergence to one of the paths will occur as a consequence of the self-reinforcing pheromone deposit mechanism. In fact the more pheromone is deposited on a path, the more ants will follow the pheromone trail on that path deposing even more pheromone.

The first application of Ant Colony Optimization method, the Ant System, has been made on the optimization version of the Travelling Salesman Problem (TSP) ([4]).

In this implementation a population of virtual agents (an ant colony) is used to explore the search space (the virtual environment).

In the same fashion as the real insects, the ants are able to deposit virtual pheromone in the environment, to signal to the other ants the presence of promising solutions.

The general outline of the implemented algorithm is the following:

Algorithm 1 Ant Colony Optimization - Outline

- $1:\ Initalize Pheromone\ Trail$
- 2: while !(TerminationCondition) do
- 3: ConstructAntsSolutions
- 4: LocalSearch (Optional)
- 5: Update Pheromone Trails
- 6: end while

The design of the solution construction and pheromone update mechanism is the main point of the algorithm. Implementation details of the basic ACO system, the Ant System can be found in [3].

Algorithm structure

The proposed algorithm is an implementation of one of the extensions to the Ant Colony Optimization metaheuristic framework, the $\mathcal{MAX} - \mathcal{MIN}$ Ant System (cf. [7]). The main differences with respect to the basic ACO approach are the following:

- Only iteration best or best-so-far ants update pheromone.
- A local search after the solution generation is used to further improve the solutions found by the ants at each iteration.
- $\forall t \ \tau_{\min} < \tau_{i,j}(t) < \tau_{\max}$ Pheromone trails have explicit upper and lower limits
- Pheromone trails are re-initialized when stagnated.

The aforementioned design choice were made because:

- The initialization of the pheromone trails to their upper bound favors diversification at the beginning of each trial.
- The pheromone update rule favors exploitation of (intensification on) the best solutions at each iteration of the algorithm.
- By bounding the intensity of the pheromone trails, the probability of stagnation (i.e. all the ants converging and exploiting a single sub-optimal tour) is reduced.
- If the pheromone trails values for the solution components of a certain tour s are equal to τ_{max} , the algorithm is said to be converged.

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Algorithm 2 $\mathcal{MAX} - \mathcal{MIN}$ Ant System for TSPTW - Outline

```
1: procedure ACO(\alpha, \beta, \rho, \tau_0, q_0, n_{ants}, n_{cities}, t_{max})
                                                                                              ▶ The main procedure
Require: N - Node set
Require: E - Edge set
Require: c - Edge cost function
Require: t - Time window function
        Initalize Pheromone Trail(\tau_0, n_{cities})
        while !TerminationCondition(t_{max}) do
3:
            for all Ant k do
 4:
                ConstructSolution(\alpha, \beta)
 5:
               Iterative Improvement ({\tt INSERT}, {\tt BEST\text{-}IMPROVEMENT})
 6:
                UpdatePheromoneTrails(\rho, q_0)
 7:
            end for
 8:
        end while
 9:
        return solution
10:
11:
12: end procedure
```

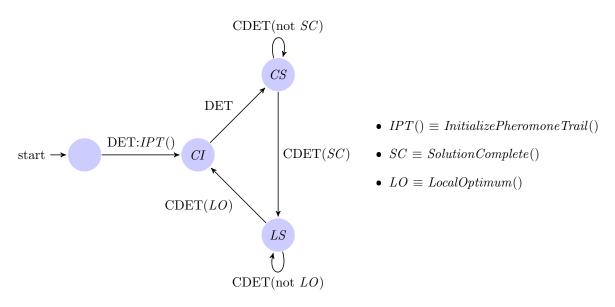


Figure 2: $\mathcal{MAX} - \mathcal{MIN}$ Ant System GLSM

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In the implementation, an instance is completely defined by:

- Cost matrix Encapsulating information on the node set N, edge set E, and weighting of each edge c.
- Time window vector Describing the time window mapping function t for each node.

Pheromone Initialization

Algorithm 3 Pheromone Initialization

```
1: procedure InitalizePheromoneTrail(\tau_0, n_{cities})
2:
          \tau_{\max} \leftarrow
 3:
          \tau_{\min} \leftarrow
          i \leftarrow 0
 4:
          j \leftarrow 0
 5:
          for i < n_{cities} do
 6:
               for j < i do
 7:
 8:
                     \tau_{ij} \leftarrow \tau_0
9:
                     \tau_{ji} \leftarrow \tau_{ij}
                     j \leftarrow j + 1
10:
                end for
11:
               i \leftarrow i+1
12:
           end for
13:
14: end procedure
```

As discussed in Introduction, the ACO methods are based on stigmergic communication among the agents by means of virtual pheromone.

While the real ants can deposit pheromone anywhere in the environment, the virtual ants may only exchange informations concerning solutions components.

For this reason, every admissible edge $e_{i,j}$ of E has an associated pheromone value $\tau_{i,j}$, that have to be initialized at the beginning of the execution of the algorithm.

The inizialization value τ_0 is a parameter of the algorithm, for the $\mathcal{MAX} - \mathcal{MIN}$ Ant System $\tau_0 = \tau_{i,j}(0) = \tau_{\max}$.

Solution construction

Algorithm 4 Solution Construction

```
1: procedure ConstructSolution(\alpha, \beta)
                                                                                                   ▶ The main procedure
                                                                      \triangleright s_i represes the i^{th} component of the solution
2:
                                                                                   ▶ Every solution starts at the depot
3:
        s_0 \leftarrow 0
       s_1 \leftarrow RandomCitySelection()
                                                                                  ▶ Random choice of the starting city
 4:
       i \leftarrow 1
5:
       while !SolutionComplete() do
 6:
            s_i \leftarrow RouletteWheelSelection()
                                                             \triangleright k stochastically chosen according to the probability
   distribution defined by 3
           i \leftarrow i + 1
8:
        end while
10: end procedure
```

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The solution construction process, used by every ant k in the system, consist of a probabilistic selection of solution components. Every edge $e_{i,j}$ has a selection probability $p_{i,j}^k(t)$ (also called transition probability) defined as follows:

$$p_{i,j}^k(t) = \begin{cases} \frac{[\tau_{i,j}(t)]^{\alpha} \cdot [\eta_{i,j}]^{\beta}}{\sum_k \in A(s_i)[\tau_{k,j}(t)]^{\alpha} \cdot [\eta_{k,j}]^{\beta}} & j \in A(s_i) \\ 0 & \text{otherwise} \end{cases}$$
(3)

As one can see in 3, the transition probability is determined by a constant, locally available heuristic information $\eta_{i,j}$ and by the time varying pheromone trail $\tau_{i,j}(t)$. This probability is defined on the set $A(s_i)$ of available (i.e. not yet visited) cities while visiting solution component s_i . The value of the parameters α and β determines the relative importance of the heuristic information and the pheromone trail, respectively

Admissible heuristics

The heuristic component $\eta_{i,j}$ is used to guide the selection of solution components towards those components that are included in optimal solution.

Dorigo et al, 1996 The heuristic originally proposed by Dorigo et al, in [4], for the TSP problem is:

$$\eta_{i,j} = \frac{1}{c(e_{i,j})} \tag{4}$$

The main idea behind this heuristic is that, if the selection process tends to select, at each step, the shortest connection between the current node and the following, the built tour should be of the shortest length. This heuristic is cited for explanation purposes, even though it cannot be used for the TSPTW problem, since it will guide the exploration only towards shortest solution, without taking into account the presence of the time windows.

Cheng and Mao, 2007 The local heuristics used in [1] are similar to that proposed by Gambardella et al. [5] in their multiple ant colony system (MACS) designed to solve the vehicle routing problem with time windows (VRPTW).

$$[\eta_{i,j}]^{\beta} = [g_{i,j}]^{\beta} \cdot [h_{i,j}]^{\gamma} \tag{5}$$

The two components $g_{i,j}$ and $h_{i,j}$, are designed, respectively, to avoid lateness (that is, arriving in the node where the time windows is already terminated) and waiting times (i.e. arriving in the node before the time windows open).

Lateness avoidance

$$g_{i,j} = \begin{cases} \frac{1}{1+e^{\delta \cdot (G_{i,j}-\mu)}} & G_{i,j} = b_j - t_j \ge 0\\ 0 & \text{otherwise} \end{cases}$$
 (6)

where

- $G_{i,j} = b_j t_j$ Slack corresponding to the time window j while being in node i
- t_i Arrival time at node i
- b_i Closing time of time window i
- $G(i) = \{k \mid G_{i,k} \ge 0\}$ Set of feasible neighbors of node i (i.e. such that node k is reached earlier than its closing time)
- $\mu = \frac{1}{|G(i)|} \sum_{j \in G(i)} G_{i,j}$ Average slack
- δ Parameter to control the slope of the sigmoidal function

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Waiting time avoidance

$$h_{i,j} = \begin{cases} \frac{1}{1 + e^{\lambda \cdot (H_{i,j} - v)}} & H_{i,j} = t_j - a_j \ge 0\\ 0 & \text{otherwise} \end{cases}$$
 (7)

where

- $H_{i,j} = t_j a_j$ Waiting time corresponding to the time window j while being in node i
- t_i Arrival time at node i
- a_i Opening time of time window i
- $H(i) = \{k \mid H_{i,k} \ge 0\}$ Set of non-waiting neighbors of node i (i.e such that node k is reached within the time window)
- $v = \frac{1}{|H(i)|} \sum_{j \in H(i)} H_{i,j}$ Average waiting time λ Parameter to control the slope of the sigmoidal function

Lopez-Ibanez and Blum, 2009 The approach used in [6] is instead, to perform a linear combination, based on λ_i coefficients, of the normalized values of opening and closing times of the time windows and the travelling cost from one city to another.

$$\eta_{i-1,k} = \lambda_a \cdot \frac{a_{\text{max}} - a_k}{a_{\text{max}} - a_{\text{min}}} + \lambda_b \cdot \frac{b_{\text{max}} - b_k}{b_{\text{max}} - b_{\text{min}}} + \lambda_c \cdot \frac{c_{\text{max}} - c_{i-1,k}}{c_{\text{max}} - c_{\text{min}}}$$
(8)

where

- a_i Opening time of time window i
- $a_{\max} = \max_{j \in N(i)} a_j$ Maximum time window opening time in the neighborhood of node i
- $a_{\min} = \min_{i \in N(i)} a_i$ Minimum time window opening time in the neighborhood of node i
- b_i Closing time of time window i
- $b_{\max} = \max_{j \in N(i)} b_j$ Maximum time window closing time in the neighborhood of node i
- $b_{\min} = \min_{j \in N(i)} b_j$ Minimum time window closing time in the neighborhood of node i
- $c_{i,j}$ Travelling cost from node i-j
- $c_{\text{max}} = \max_{i} c_{i,j}$ Maximum travelling cost from node i
- $c_{\min} = \min_i c_{i,j}$ Minimum travelling cost from node i
- $\lambda_a, \lambda_b, \lambda_c$ s.t. $\lambda_a + \lambda_b + \lambda_c = 1$ Randomly selected weights

In this implementation, the heuristic information will be computed according to [6]

Pheromone Trails Update

As discussed in Algorithm structure, the pheromone update will be made by a single ant, being either the one who found the best solution in the current iteration:

$$\Delta \tau_{i,j}^{Bi} = \begin{cases} \frac{1}{T_{\text{di}}^{\text{Bi}}} & e_{i,j} \in T^{\text{Bi}} \\ 0 & \text{otherwise} \end{cases}$$
 (9)

Or the one having found the global best (best-so-far) solution:

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Algorithm 5 Pheromone Trails Update

```
1: procedure UPDATEPHEROMONETRAILS(\rho, q_0)
                                                                                                                                         ▶ The main procedure
 2:
 3:
           j \leftarrow 0
 4:
           for i < n_{cities} do
                 for i < i do
 5:
                      if Random() < q_0 then
 6:
                           \tau_{ij} \leftarrow (1 - \rho) \cdot \tau_{ij} + \Delta \tau_{i,j}^{Bi}
 7:
 8:
                           \tau_{ij} \leftarrow (1 - \rho) \cdot \tau_{ij} + \Delta \tau_{i,j}^{Bo}
9:
10:
11:
                      if \tau_{ij} < \tau_{\min} then
                            \tau_{ij} \leftarrow \tau_{\min}
12:
13:
                      end if
                      if \tau_{ij} > \tau_{\max} then
14:
15:
                           \tau_{ij} \leftarrow \tau_{\max}
16:
                      end if
17:
                      \tau_{ji} \leftarrow \tau_{ij}
                      j \leftarrow j + 1
18:
                 end for
19:
                 i \leftarrow i + 1
20:
           end for
21:
22: end procedure
```

$$\Delta \tau_{i,j}^{Bo} = \begin{cases} \frac{1}{T_d^{\text{Bo}}} & e_{i,j} \in T^{\text{Bo}} \\ 0 & \text{otherwise} \end{cases}$$
 (10)

where

- $e_{i,j}$ Edge connecting node i and j
- T_d^i Complete tour duration of tour i
- ullet T^{Bi} Best tour of the current iteration
- T^{Bo} Best tour overall

Provided that the best solution is known, the bounds on the pheromone values can be estimated as:

$$\hat{\tau}_{\text{max}} = \frac{1}{\rho \cdot T_d^{\text{Go}}} \qquad \hat{\tau}_{\text{min}} = \frac{\hat{\tau}_{\text{max}}}{a} \tag{11}$$

Results discussion

By looking at tables ??, ??, ??, ?? one can see that:

- For some instances (e.g. n80w20.002, n80w20.003) the algorithm are not able to converge to a feasible solution, as shown in the corresponding boxplots, since the PRPD distribution is centered around 12000-15000, thus indicating the presence of at least 1 constraint violations in most of the cases.
- For some other instances (e.g. n80w20.004, n80w20.005) the algorithms are able to converge to feasible solutions and to the best-known one, but having a right-skewed distribution towards higher values of PRPD.

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- For the remaining instances, except for some outlier values, the algorithms are able to converge to the best-known solution in most of the runs, even though the average PRPD is not closer to 0. This is due to the fact that the mean of a distribution is sensible to outliers and the penalisation for a constraint violations is extremely high when compared to the mean value.
- The algorithm ordering in terms of runtimes is s.tie < p.tie < p.tie < p.tei < s.tei for the n80w20.X instances while s.tie < p.tei < s.tei < p.tie for n80w200.X ones. The choice to explore the Insert Neighborhood before the Exchange one allows to reduce the computation time for the n80w20.X instances, with a similar solution quality.
- The algorithms are more effective on the n80w200.X instances then the n80w20.X once, since they have a lower percentage of infeasible runs and a lower PRPD.
- The standard variable neighborhood descent with Transpose-Insert-Exchange neighborhood chain (s.tie) outperforms all the other algorithms in terms of solution quality and runtime.
- Tables ??, ??, ??, ??, ??, ??, ??, ??, ?? contain, in any case, p-values considerably smaller than the significance level ($\alpha = 0.05$).
 - This implies that the null hypothesis corresponding to the equality of the median values of the differences of the two distributions can be rejected, hence assessing the existence of a statistically significant difference among the solution quality generated by analyzed algorithms.
- By looking at the Cpu time, one can see that the instances n80w20.X have generally lower runtimes than the n80w200.X ones. They can then be considered, with respect to the variable neighborhood descent algorithms, simpler (quickier to solve) instances with respect to the latter.

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Problem 2

Iterative improvement algorithms

Problem statement

Implement iterative improvement algorithms with:

- first-improvement
- best-improvement

pivoting rule for each of the three neighborhoods: transpose, exchange, and insert.

As a starting solution for iterative improvement, consider a random permutation, that is, use the method "Uninformed Random Picking" (see slides of lectures). Bonus points will be awarded for also considering an insertion heuristic as an alternative to random initialization.

- 1. Run the 6 resulting iterative improvement algorithms (all combinations of the two pivoting rules and the three neighborhoods) on each of the instances. Repeat each run 100 times with different seed for the random number generator.
- 2. Compute the following statistics for each of the 6 iterative improvement algorithms and each instance:
 - Percentage of runs with constraint violations
 - Mean penalised relative percentage deviation
 - Mean computation time
- 3. Produce boxplots of penalised relative percentage deviation and computation time per instance.
- 4. Determine using statistical tests (in this case, the Wilcoxon test), whether there is a statistically significant difference between the quality of the solutions generated by the different algorithms. In particular, compare best vs. first-improvement for each neighborhood, and exchange vs. insertion for each pivoting rule.

Metric definitions

For each algorithm k, applied on instance i, using different randomly generated seeds one have to compute:

- Number of constraint violations
- Penalised relative percentage deviation (PRPD)
- Computation time (CPU time)

In order to perform a statistical analysis of the results, each algorithm k is launched 100 times on the same instance, computing the following statistics:

- Percentage of infeasible solutions (0.x has to be interpreted as x%)
- Average Penalised relative percentage deviation.
- Average Computation time (CPU time).

For each instance i, the distributions of PRPD and Cpu Times are displayed using box plots and the Wilcoxon signed rank test is performed, in order to assess the existence of a statistically significant difference among the results obtained by the different algorithms on the same instance.

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Constraint Violations In the standard formulation of the TSP problem, a solution to the problem is represented by a permutation of the different entities (solution components), that the hypothetical travelling salesman has to visit.

The best solution for the problem is the permutation that minimizes the total travelling time (distance) among the cities. The presence of time windows introduce an additional constraint on the feasibility of the solution.

In fact, each solution component has an associated time window within which it has to be visited in order to guarantee the feasibility of the tour.

Arriving in a (city) before the opening of the corresponding time window involves a delay in the total travelling time (to wait for the time window to open) whereas the arrival after the closure of the time windows will generate a constraint violation.

Thus, a solution is feasible if and only if all the time windows constraints are met, or in other words, if there are no constraint violations.

In this case, the best solution is the feasible solution which minimizes the total travel time.

Penalised Relative Percentage Deviation The penalised relative percentage deviation (PRDP from now on) is a measure of the solution quality, with respect to the best known solution for the instance, taking into account a strong penalisation for the violation of constraints. The PRPD is computed as follows:

$$pRPD_{kri} = 100 \cdot \frac{(f_{kri} + 10^4 \cdot \Omega_{kri}) - best_i}{best_i}$$
(12)

Runtime The runtime is a measure of both the quality and the time complexity of the algorithm.

It is measured using the function int clock_gettime(clockid_t clk_id, struct timespect *tp) from the time.h library.

The parameter clk_id=CLOCK_PROCESS_CPUTIME_ID, is used to read the values from an high-resolution timer provided by the CPU for each process.

The runtime is computed (using the user defined function ComputeRunTime) as the difference, with a resolution of 10^-9 s, from the time obtained using clock_gettime at the beginning and the one obtained at the end of the simulation.

Simulated Annealing

```
Algorithm 6 Simulated Annealing TSPTW
  procedure Simulated Annealing (\tau_0, n_{cities})
Require: Annealing schedule
      s \leftarrow InitialSolution()
                                                                                  ▶ Heuristic or random permutation
      T \leftarrow T_0
      while ! TerminationCondition() do
          s' \leftarrow ProposalMechanism()
                                                                          \triangleright (Often) Uniform random choice in N(s)
          if AcceptanceCriterion(T) then
                                                                                       ▷ (Often) Metropolis condition
              s \leftarrow s'
          end if
          T \leftarrow Update(T)
                                                                                                          \triangleright T_{i+1} = \alpha \cdot T_i
      end while
  end procedure
```

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Algorithm 7 Initial solution

procedure Initial Solution end procedure

Algorithm 8 Termination condition

procedure Termination condition end procedure

$$P(s, s', T) = \begin{cases} 1 & f(s) < f(s') \\ 1 & f(s) = f(s') \land \Omega(s) < \Omega(s') \\ e^{\frac{f(s) - f(s')}{T}} & \text{otherwise} \end{cases}$$
 (13)

Results discussion

By looking at tables ??, ??, ??, ?? ??, ?? on can see that:

- The neighborhood type has a strong influence on the both the time complexity of the algorithm and the generated solution quality. This is due to the size of the different neighborhoods (n = 80):
 - Transpose (n-1)
 - Exchange $\frac{n\cdot (n-1)}{2}$
 - Insert $(n-1)^2$

The different size of the neighborhoods corresponds to different degrees of exploration (diversification).

- Transpose and Exchange neighborhoods have smaller runtimes but a percentage of infeasible runs equal to 1. Both the algorithm do not allow to find a feasible solution but the Exchange algorithm constructs solutions with a better quality (reduced, but not yet null, constraint violations and total travel time).
- Insert is the only neighborhood type that allows to generate solutions that are both feasible and closer to the global optima.
- The first-improvement pivoting rule is generally slower than the best-improvement one, when considering the same neighborhood type. This is due to the fact that, with the first-improvement pivoting rule, smaller improvement are made to the solution at each iteration, thus requiring and higher number of iteration to converge to a local optima, with respect to the case where the best improvement is chosen at each time step.
- The quality of the solutions generated using the first-improvement pivoting rule is slightly better than those generated using the best-improvement one.
- Tables ??, ??, ??, ??, ??, ??, ??, ??, ?? contain, in any case, p-values considerably smaller than the significance level ($\alpha = 0.05$).

Algorithm 9 Proposal mechanism

procedure Proposal Mechanism end procedure

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Algorithm 10 Acceptance Criterion

procedure Acceptance criterion end procedure

Algorithm 11 Update according to annealing schedule

 $\begin{aligned} & \mathbf{procedure} \ \ \mathbf{UPDATE}(T) \\ & T \leftarrow \alpha \cdot T \\ & \mathbf{end} \ \mathbf{procedure} \end{aligned}$

This implies that the null hypothesis corresponding to the equality of the median values of the differences of the two distributions can be rejected, hence assessing the existence of a statistically significant difference among the solution quality generated by analyzed algorithms.

• By looking at the Cpu time, one can easily see that the instances n80w20.X have lower runtimes than the n80w200.X ones. They can then be considered, with respect to the iterative improvement algorithms, simpler instances with respect to the latter.

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Conclusions

By combining the results from the previous analysis:

- The Iterative Improvement algorithms based on Transpose and Exchange neighborhoods do not allow to find feasible solutions hence they should not be considered for a practical application.
- On the other hand, the solution quality generated by the Iterative Improvement algorithm with the Insert neighborhood is similar to those generated by the VND algorithms, regardless of the instances.
- On this set of instances, the VND algorithms have a lower runtime than the Iterative Improvement one using Insert neighborhood, hence being similar the resulting solution quality, they should be preferred to the Iterative Improvement ones.
- The algorithm that showed the best performances in terms of solution quality and runtime is the Standard Variable Neighborhood Descent with Transpose-Insert-Exchange neighborhood chain.
- The usage of average statistics as metrics to measure the quality of the algorithms is strongly biased by the presence of outliers (penalisation, in this case).

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