

Chapter 1

Literature Review

(TODO) Present a survey of your main approach and an overview of the approaches proposed previously for solving the problem dealt with in this work

(TODO) Identify the practical and research motivation of this work and the literature gaps

(TODO) How convincing is the authors' argument? (Critical response - comparisons with other research, strengths or weaknesses but in relation to your research)

1.1 Optimisation in Air Travel

In this section, we discuss some common challenges faced by airline companies and demonstrate the importance of optimisation in decision-making. The goal is to provide insight into some important optimisation problems, underscoring their importance for the success and competitiveness of airline companies.

1.1.1 Fleet Assignment Problem

The Fleet Assignment Problem (FAP), as discussed in [1] involves assigning different types of aircraft, each with specific capacities, to flights based on their capabilities, operational costs, and revenue potential. This decision greatly influences airline revenues and is a vital part of the overall scheduling process. The complexity of FAP is driven by the large number of flights an airline manages daily and its interdependencies with other processes like maintenance and crew scheduling.

1.1.2 Crew Scheduling Problem

The Crew Scheduling Problem (CSP), as discussed in [2], involves assigning crews to a sequence of tasks, each with defined start and end times, with the primary objective of ensuring that all tasks are covered while adhering to regulations on maximum working hours for crew members.

This problem is particularly critical for low-cost carriers, for instance in the United Kingdom in 2023, the low-cost carriers comprise 48% of the scheduled capacity (total number of seats offered) [3], which rely heavily on optimised crew schedules to maintain competitiveness. Efficient crew scheduling is essential not only for low cost carriers and for cost minimisation but also for ensuring operational reliability and flexibility in response to unexpected disruptions. [4]

1.1.3 Disruption Management

Disruptions in airline operations, as noted in [5], can occur due to various factors, including crew unavailability, delays from air traffic control, weather conditions, or mechanical failures. Given that flight schedules are typically planned months in advance [6], effective disruption management is crucial to minimise the impact on passengers and overall airline operations.

The two main drivers of disruption management are aircraft and crew recovery.

- Aircraft recovery: Reassigning aircraft to flights after disruption by taking care of schedules, airports availability and maintenance. Optimisation tools help manage the complex logistics of matching available aircraft with rescheduled flights, considering factors like airport availability and maintenance requirements. This ensures that the revised schedules are as efficient and practical as possible.
- Crew recovery: reassigning crew members to flights by respecting all flights are staffed appropriately. Optimisation tools are used to adjust crew schedules, taking into account factors such as legal working hours, crew availability, and the need to cover all flights efficiently. These tools help in developing feasible and compliant crew rosters that adapt to the new flight schedules.

These optimisation strategies, supported by advanced software, for instance [7] and [8], are crucial for reducing the impact of disruptions and boosting operational resilience in the airline industry.

1.1.4 Airline adaptation to new demand

Airlines companies must continuously adapt their schedules to meet evolving market demands, particularly with the growing dominance of leisure travel over business travel, which has introduced new patterns of demand seasonality, especially in Europe as shown on Figure 1.1. This seasonality poses a challenge for airlines as they have to balance high demand during peak seasons with the risk of underutilisation during off-peak times.

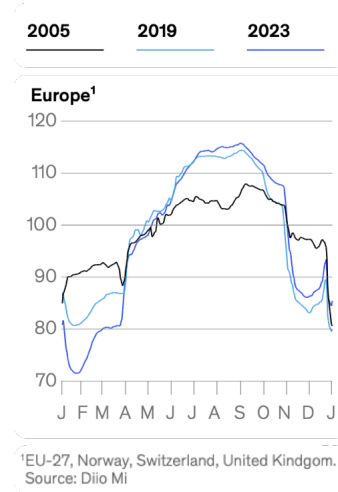


FIGURE 1.1: European demand seasonality [9]

Since travel demand varies throughout the year, seasonal-wise, airlines use a variety of techniques to achieve operational efficiency while maximising revenue [9]. The seats that airlines book are nearly 65% more in August than they do in February when summer peak demand skyrocketed. They make the required allowance for additional aircraft and crew by optimisation models that specify priority routes and requirements for additional flights, alongside effective crew rotation management to have everything go smoothly due to the heightened demand of resources.

In contrast, winter months pose a different type of problem: demand drops, meaning potential underutilisation of aircraft. To do this, airlines are known to turn to ACMI leasing (agreement between two airlines, where the lessor agrees to provide an aircraft, crew, maintenance and insurance [10]) during periods of low demand to temporarily

reduce fleet size by outsourcing their capacity. Parallel to this, they also increase maintenance activities and incentivise crews to take holidays or undergo training to maximise productivity across the operation. Equally, on a year-round basis, airlines apply dynamic pricing algorithms to vary fares in reaction to real-time demand patterns. In high-demand summer months, fares are tactically set so as to maximise revenues from travelers willing to pay more, while in winter, pricing strategies are aimed at stimulating demand with fare reductions to fill seats that otherwise would have gone empty and improve overall aircraft utilisation. Such adaptive strategies are critical to the airlines for effectively beating the seasonal ebbs and flows in the travel industry.

1.2 Traveling Salesman problem and its adaption

The Traveling Salesman Problem is a well known problem in the Operational Research and Computer Science area. The basic version of the TSP is to find the best roundtrip for a salesman that has to travel around a given number of cities while minimising the overall journey's distance. This problem is characterised as \mathcal{NP} -Hard [11]. This means that there is no known polynomial-time algorithm that can solve all instances of the problem efficiently. In terms of time complexity, if we were to solve it exploring all the possible solutions the time complexity would have been $\mathcal{O}(\frac{(n-1)!}{2})$ where n represents the number of cities.

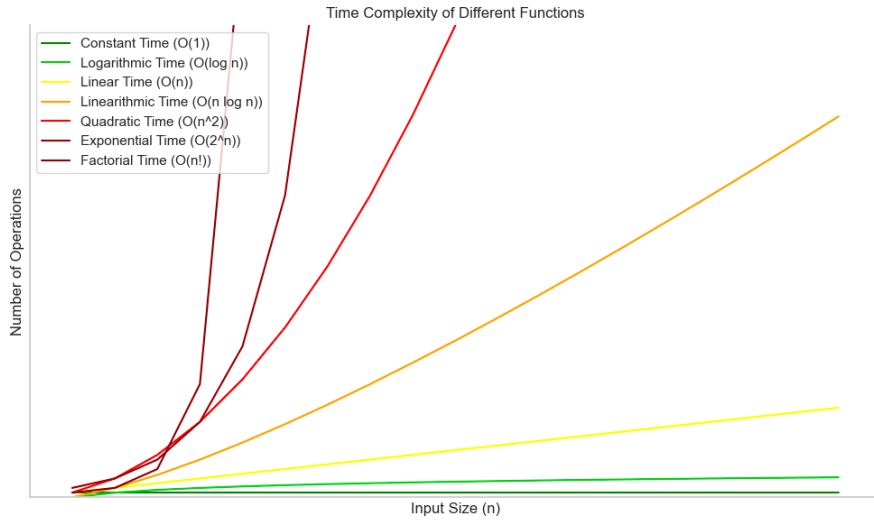


FIGURE 1.2: Time complexity of different functions [12]

On Figure 1.2, different time complexity are compared and the factorial time complexity is the worst. That means that these kinds of \mathcal{NP} -Hard problem are typically not solved exploiting all the search area but using heuristics algorithms. Heuristics solutions do not guarantee to find the absolute optimal solution but can find near-optimal solutions in a much more reasonable times.

The TSP has been studied extensively, not least because many variants can be derived from it:

- Symmetric TSP (STSP): The distance between cities are symmetric, meaning that the distance to travel from city A to city B is the same as from city B to city A.

- **Assymmetric TSP (ATSP):** The distance between cities are assymmetric, meaning that the distance to travel from city A to city B is different than the distance to travel from city B to city A. [13]
- **Multiple TSP (mTSP):** Instead of one salesman, multiple salesman are starting from one city visit all the cities such that each city is visited exactly once. [14]
- **Time Window TSP (TWTSP):** Each city has to be visited in a defined time slot. [15]
- **Price-collection TSP (PCTSP):** Not all the cities have to be visited, the goal is to to minimise the overall traveler's distance while maximising the price collected earned when visiting a city. [16]
- **Stochastic TSP (STSP):** The distances between the cities or the cost of travels are stochastic (i.e random variables) rather than deterministic. [17]
- **Dynamic TSP (DTSP):** The problem can change over the times, that means that new cities can be added or distances between cities can change while the salesman has already started his journey. [18]
- **Generalised TSP (GTSP):** The cities are grouped into clusters, the goal is to visit exactly one city from each cluster. [19]
- **Open TSP (OTSP):** The traveler does not have to end his journey at the starting city. [20]

Multiple algorithms have been developed to address these TSP variants, we can classify them into two major categories:

- **Exact Algorithms:** These algorithms aim to find the optimal solution to the TSP by exploring all possible routes or by using mathematical techniques to prune the search space efficiently. Examples include:
 - **Branch and Bound:** This method systematically explores the set of all possible solutions, using bounds to eliminate parts of the search space that cannot contain the optimal solution. It is often used for smaller instances of TSP due to its computational intensity. [21]
 - **Cutting Planes:** This technique adds constraints (or cuts) to the TSP formulation iteratively to remove infeasible solutions and converge to the optimal solution. This approach is particularly effective for symmetric TSPs. [22]

- **Dynamic Programming:** Introduced by Bellman, this approach breaks down the TSP into subproblems and solves them recursively, which is highly effective for specific TSP variants, though its complexity grows exponentially. [23]
- **Approximation and Heuristic Algorithms:** These algorithms are designed to find near-optimal solutions within a reasonable time frame, especially for large-scale problems where exact methods are computationally infeasible. Examples include:
 - **Greedy Algorithms:** These algorithms make a series of locally optimal choices in the hope of finding a global optimum. An example is the Nearest Neighbor algorithm, which selects the nearest unvisited city at each step. [24]
 - **Genetic Algorithms:** Inspired by the process of natural selection, these algorithms evolve a population of solutions over time, using operations such as mutation and crossover to explore the solution space. [25]
 - **Simulated Annealing:** This probabilistic technique searches for a global optimum by allowing moves to worse solutions based on a temperature parameter that gradually decreases. It is particularly useful for escaping local optima. [26]
 - **Ant Colony Optimization:** This metaheuristic is inspired by the foraging behavior of ants and uses a combination of deterministic and probabilistic rules to construct solutions, gradually improving them through pheromone updates. [27]

Some TSP problems (or its variants) have been solved using other algorithms, hence they are less traditionnal than those mentionned.

1.3 The Monte Carlo Tree Search algorithm

The Monte Carlo Tree Search (MCTS) algorithm can be characterised less traditional than the previously enounced method in Section 1.2 to solve TSP because MCTS is typically used in games. MCTS' (and its variants) have been successfully implemented across a range of games, such as Havannah [28], Amazons [29], Lines of Actions [30], Go, chess, and Shogi [31], establishing it as the state-of-the-art method for many of these games [32], [33], [34]. It is widely use in board games and has been really popular when Google DeepMind developed AlphaGo. AlphaGo is a software that was created to beat the best Go's player in the world.

Go is an ancient board game from China where two players take turns placing black or white stones on a grid. The goal is to capture territory by surrounding empty spaces or the opponent's stones. Despite its simple rules, Go is incredibly deep and complex, with countless possible moves and strategies. It is known for its balance between intuition and logic, hence it has been a significant focus of artificial intelligence research ,[35]. In 2016, Lee Sedol [36] - the best Go's player in the world has been beaten by AlphaGo 4-1 [37].

MCTS with policy and value networks are at the heart of AlphaGo's decision-making process, enabling AlphaGo's to pick the optimal moves in the complex search of Go. [38]

1.3.1 Overview

The MCTS' process is conceptually straightforward. A tree is built in an incremental and assymatric manner (Figure 1.3). For every iteration, a selection policy is used to determine which node we have to select in the tree to perform simulations. The selection policy, typically balances the exploration i.e. look into part of the tree that have not been visited yet and the exploitation i.e. look into part of the trees that appear to be promising. Once the node is selected, a simulation i.e. a sequence of available actions, based on a simulation policy, are applied from this node until a terminal condition is reached e.g no further actions are possible. [39]

To ensure that the reader understands the various stages of the Monte Carlo Tree Search Algorithm, we will begin by looking at a detailed example. This example will illustrate

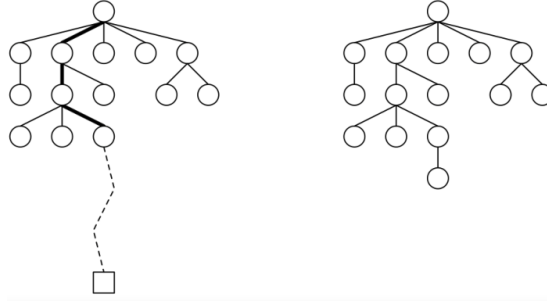


FIGURE 1.3: Assymetrical growth of MCTS - Simulation and Expansion - [40]

each component of the algorithm in action. We will then generalise the principles discussed, as the basic methodology of this paper is based on the application of the MCTS algorithm.

1.3.2 Example

Let's say we are given a maximisation problem. When starting the game, you have two possible actions a_1 and a_2 from the node $S_0^{0,0}$ in the tree \mathcal{T} . Every node is defined like so: $S_i^{n_i, t_i}$ where n_i represents the number of times node i has been visited, t_i the total score of this node. Furthermore, for every node - we can compute a selection metric, for instance the $UCB1$ value: $UCB1(S_i^{n_i, t_i}) = \bar{V}_i + 2\sqrt{\frac{\ln N}{n_i}}$ where $\bar{V}_i = \frac{t_i}{n_i}$ represents the average value of the node, n_i the number of times node i has been visited, $N = n_0$ the number of times the root node has been visited (which is also equal to the number of iterations).

Before the first iteration, none node have been visited - $\forall i \in \mathcal{T}, S_i^{0,0}$. At the beginning

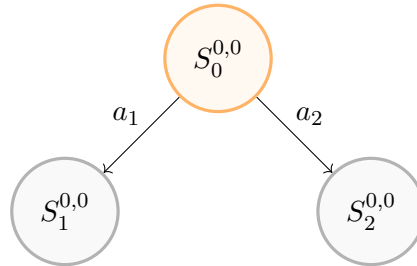


FIGURE 1.4: Selection - I1

of I1, we then have to choose between these two child nodes (or choose between taking a_1 or a_2). We then have to calculate the $UCB1$ value for these two nodes and pick the node that maximises the $UCB1$ value (as we are dealing with a maximisation problem).

In Figure 1.4, neither of these have been visited yet so $USB(S_1^{0,0}) = UCB1(S_2^{0,0}) = \infty$. Hence we decide to choose randomly $S_1^{0,0}$.

$S_1^{0,0}$ is a leaf node that has not been visited - then we can simulate from this node i.e. selecting actions from this node based on the simulation policy to a terminal state as shown on Figure 1.5:

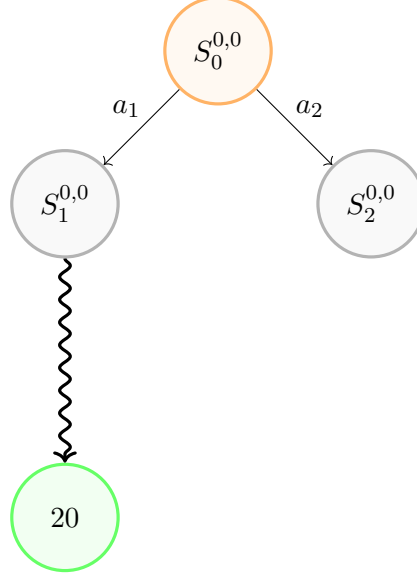


FIGURE 1.5: Simulation - I1

The terminal state has a value of 20, we can write that the rollout/simulation from node $S_1^{0,0}$ node is $\mathcal{R}(S_1^{0,0}) = 20$. The final step of $I1$ is backpropagation. Every node that has been visited in the iteration is updated. Let $\mathcal{N}_{\mathcal{R},j}$ be the indexes of the nodes visited during the j -th iteration of the MCTS:

- Before backpropagation:

$$\forall i \in \mathcal{N}_{\mathcal{R},j}, S_{i,old}^{n_i,t_i} \quad (1.1)$$

- After backpropagation:

$$\forall i \in \mathcal{N}_{\mathcal{R},j}, S_{i,new}^{n_i+1,t_i+\mathcal{R}(S_{i,old}^{n_i,t_i})} \quad (1.2)$$

We can then define a backpropagation function:

$$\begin{aligned} \mathcal{B} : \mathcal{N}_{\mathcal{R},j} &\rightarrow \mathcal{N}_{\mathcal{R},j} \\ S_i^{n_i,t_i} &\mapsto S_i^{n_i+1,t_i+\mathcal{R}(S_i^{n_i,t_i})} \end{aligned}$$

Then, back to our example on Figure 1.6 we update the nodes $\mathcal{B}(S_1^{0,0}) = S_1^{1,20}$ and $\mathcal{B}(S_0^{0,0}) = S_0^{1,20}$.

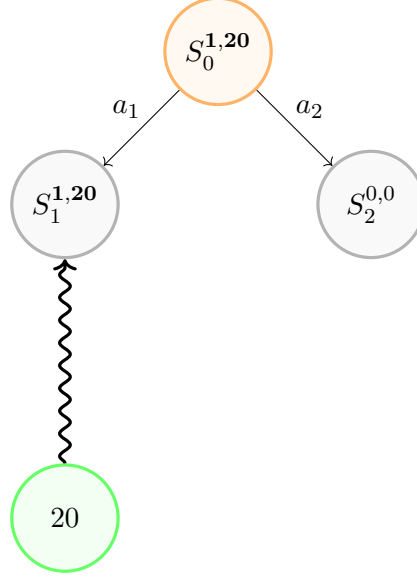


FIGURE 1.6: Backpropagation - I1

The fourth phase of the algorithm have been done for $I1$. We can then start the 2^{nd} iteration $I2$. On Figure 1.7, we can either choose a_1 or a_2 . When a child node has not

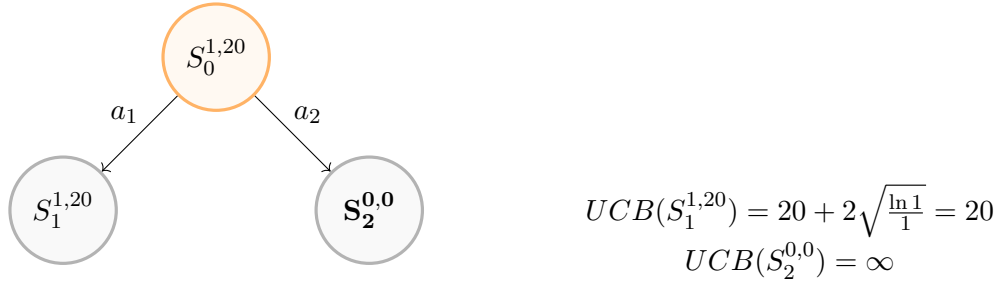


FIGURE 1.7: Selection - I2

been visited yet, you pick this node for the Selection or you can compute the $UCB1$ value, it leads to the same conclusion.

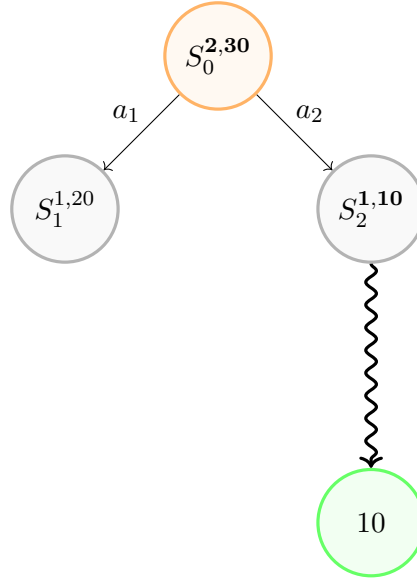


FIGURE 1.8: Simulation and Backpropagation - I2

We can then simulate (Figure 1.8) from the chosen node $S_2^{0,0}$ and $\mathcal{R}(S_2^{0,0}) = 10$ and backpropagate all the visited nodes: $\mathcal{B}(S_2^{0,0}) = S_2^{1,10}$ and $\mathcal{B}(S_1^{1,20}) = S_0^{2,30}$. We now start the 3rd iteration, based on the *UCB1* score we decide to choose a_1 .

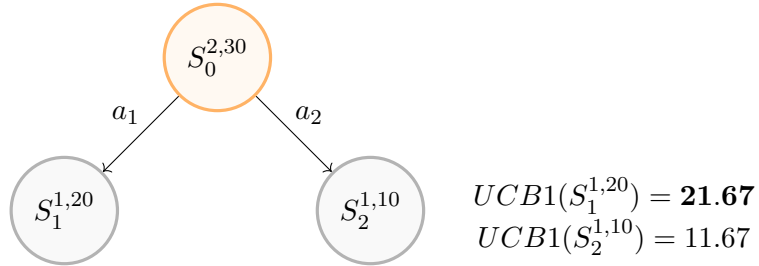


FIGURE 1.9: Selection - I3

$S_1^{1,20}$ is a leaf node and has been visited so we can expand this node.

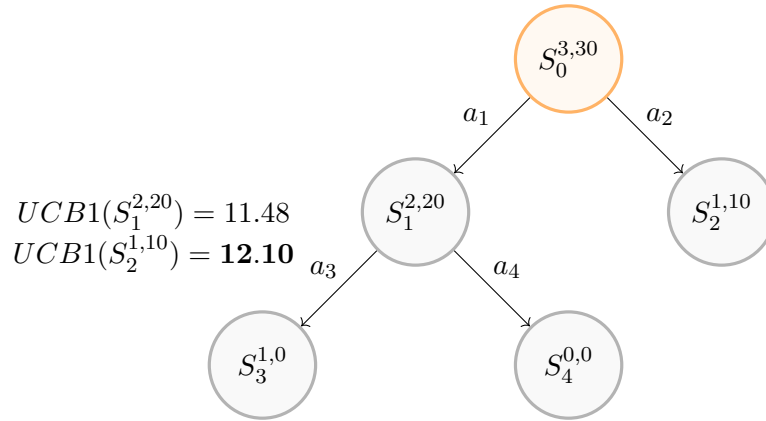


FIGURE 1.10: Selection and Expansion - I3

Based on $UCB1$ score we decide to simulate from $S_3^{0,0}$ on Figure 1.11

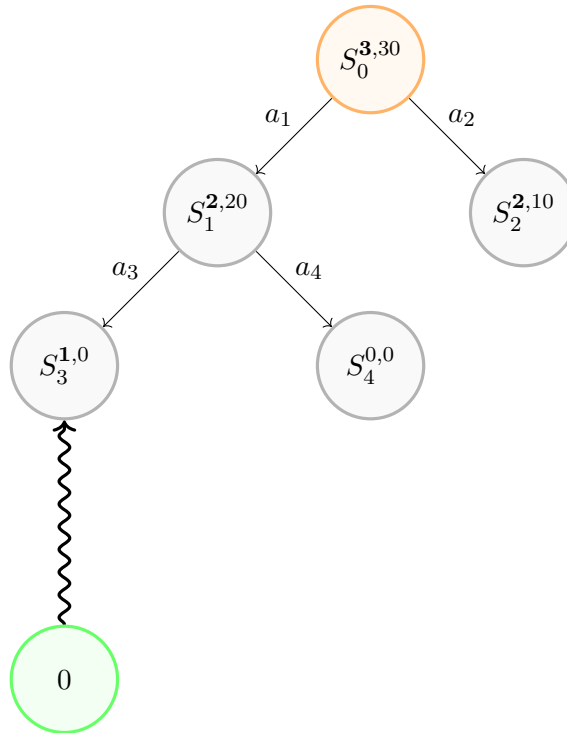


FIGURE 1.11: Simulation and Backpropagation - I3

Let's do the fourth iteration $I4$ represented on Figure 1.12:

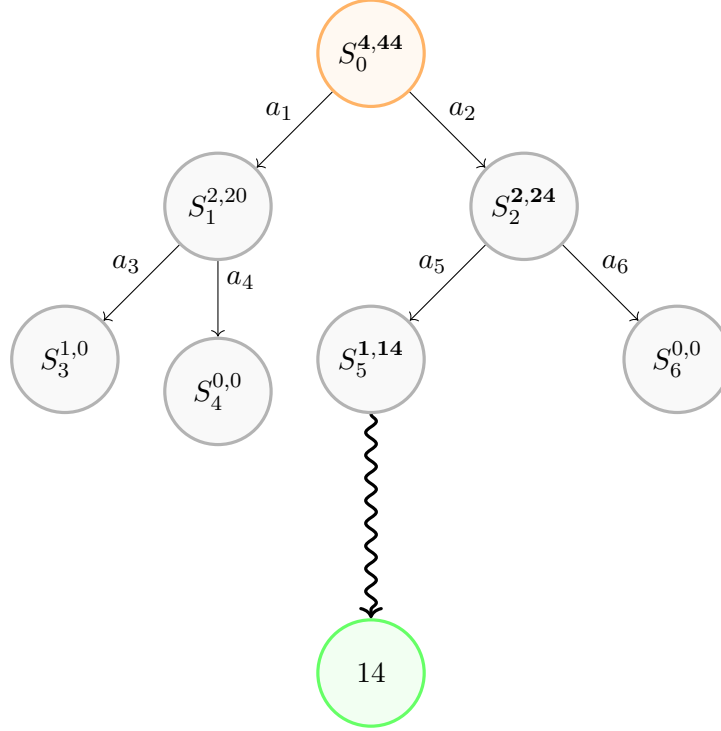


FIGURE 1.12: Selection - Simulation - Backpropagation - $I4$

The MCTS algorithm can be either stopped because you are running out of time or because you have no more available actions. For instance, if we were to stop at this stage of the algorithm, the best action to undertake is a_2 because it has the higher average value: $\bar{V}_1 = \frac{20}{2} \leq \bar{V}_2 = \frac{24}{2}$.

1.3.3 The different parameters in the MCTS

1.3.4 Selection policy

[41]

- **Upper Confidence Bound (UCB):**

- *Description:* UCB is a popular selection policy in MCTS that balances exploration and exploitation using a mathematical formulation that considers both the average reward of a node and the uncertainty of that reward.
- *Trade-offs:*

- * **Exploration vs. Exploitation:** UCB adjusts the balance between exploring less-visited nodes and exploiting nodes with high rewards.
- * **Parameter Sensitivity:** The performance of UCB depends on the constant C_p in its formula, which controls the level of exploration.
- * **Children's Count:** UCB can lead to varying numbers of children being explored, depending on the setting of C_p .

- **UCB1-Tuned:**

- *Description:* A variation of UCB that dynamically adjusts the exploration term based on the variance of rewards, making it more adaptive to different scenarios.
- *Trade-offs:*
 - * **Adaptivity:** UCB1-Tuned can adapt to the variance in the rewards, potentially leading to better performance in complex environments.
 - * **Computational Cost:** The added complexity in adjusting the exploration term may lead to higher computational costs.
 - * **Children's Count:** This policy may result in fewer nodes being selected for expansion when the variance is low, focusing more on exploitation.

- **Single-Player (SP-MCTS):**

- *Description:* A variant of MCTS specifically designed for single-player scenarios, incorporating a third term in the UCB formula to account for the uncertainty in node values.
- *Trade-offs:*
 - * **Exploration of Uncertainty:** SP-MCTS inflates the uncertainty term for less-visited nodes, which can lead to more thorough exploration in single-player settings.
 - * **Focus on Strong Lines:** This policy tends to favor strong lines of play, potentially neglecting less promising but necessary exploratory paths.
 - * **Children's Count:** Tends to explore a wider range of children nodes, balancing between known strong strategies and potential new solutions.

- **Bayesian UCT:**

- *Description:* Bayesian UCT integrates Bayesian statistics into the selection policy, allowing for a probabilistic approach to balancing exploration and exploitation.

– *Trade-offs:*

- * **Probabilistic Exploration:** Bayesian UCT provides a more nuanced exploration strategy by considering prior knowledge and updating beliefs as more information is gathered.
- * **Complexity:** The Bayesian approach can be computationally expensive, especially in large search spaces.
- * **Children’s Count:** The number of children explored under Bayesian UCT can be influenced by the prior distributions used, potentially leading to more focused exploration in areas of high uncertainty.

1.4 Selection Policies

1.4.1 Single-Player MCTS (SP-MCTS)

Single-Player MCTS (SP-MCTS) is an adaptation of the Monte Carlo Tree Search (MCTS) algorithm specifically designed for single-player games. SP-MCTS modifies the standard Upper Confidence Bounds (UCB) formula by adding a third term to account for the possible deviation of a node’s value, adjusting the standard deviation for infrequently visited nodes to better estimate rewards.

The modified UCB formula used in SP-MCTS is:

$$rD\frac{\sigma^2}{n_i} + n_i, \quad (1.3)$$

where σ^2 is the variance of the node’s simulation results, n_i is the number of visits to the node, and D is a constant that inflates the standard deviation for less frequently visited nodes.

Key enhancements in SP-MCTS include:

- **Heuristic-Guided Default Policy:** A heuristic is used to guide simulations, improving the efficiency of the search process.
- **Meta-Search:** To avoid getting stuck in local maxima, SP-MCTS periodically restarts with different random seeds and stores the best solution across runs.
- **Maximization Tracking:** By tracking maximum simulation results, SP-MCTS ensures that strong lines of play are not overshadowed by weaker ones.

1.4.2 UCB1-Tuned

UCB1-Tuned is an enhancement of the standard UCB1 algorithm, designed to fine-tune the balance between exploration and exploitation in MCTS. This approach adjusts the exploration term based on sample variance, providing a more accurate trade-off in dynamic environments.

The UCB1-Tuned formula is:

$$\sqrt{\frac{\ln n}{n_j}} \cdot \min(1, V_j(n_j)), \quad (1.4)$$

where:

$$V_j(n_j) = \frac{1}{2} \sum_{s=1}^{n_j} (X_{j,s}^2 - X_j) + \frac{\sqrt{2 \ln t}}{s}, \quad (1.5)$$

and n_j is the number of times the machine j has been played, $X_{j,s}$ is the reward for each play, and t is the total number of plays.

Notable applications of UCB1-Tuned include:

- **Improved Exploration-Exploitation Trade-off:** UCB1-Tuned replaces the upper confidence bound term with one that accounts for variance, leading to better decision-making.
- **Domain Applications:** The UCB1-Tuned approach has been successfully applied in games like Go and real-time environments, showing superior performance compared to the standard UCB1.

1.4.3 Upper Confidence Bounds for Trees (UCT)

UCT is the foundational algorithm for MCTS, combining Monte Carlo simulations with the UCB1 algorithm for selecting actions during the search process. UCT ensures a balance between exploring new actions and exploiting known good ones.

The UCB1 formula used in UCT is:

$$X_j + C_p \sqrt{\frac{\ln N}{n_j}}, \quad (1.6)$$

where X_j is the average reward from action j , C_p is the exploration constant, N is the total number of simulations, and n_j is the number of times action j has been tried.

Core components of UCT:

- **Exploration-Exploitation Balance:** UCT employs the UCB1 formula to manage the trade-off between exploration and exploitation during tree growth.
- **Tree Growth Mechanism:** UCT builds a search tree dynamically, where nodes are expanded based on the outcomes of simulations, continuously refining the action-value estimates.

1.4.4 Bayesian UCT

Bayesian UCT introduces Bayesian methods into the UCT framework to improve the estimation of node values and their uncertainties, especially in scenarios with limited simulation trials.

The Bayesian tree policy can be represented as:

$$B_i = \mu_i + \frac{\sqrt{2 \ln N}}{n_i}, \quad (1.7)$$

where μ_i is the mean of an extremum (minimax) distribution P_i , and n_i is the number of visits to the node i .

An alternative Bayesian UCT formula is:

$$B_i = \mu_i + \sigma_i \cdot \sqrt{\frac{2 \ln N}{n_i}}, \quad (1.8)$$

where σ_i is the square root of the variance of P_i .

Key strategies in Bayesian UCT:

- **Bayesian Tree Policies:** Two tree policies are proposed—one that maximizes mean rewards and another that maximizes mean plus variance, with the latter often showing superior performance.
- **Improved Convergence:** Bayesian UCT demonstrates better convergence properties compared to standard UCT, particularly when accurate prior information is available.

1.4.4.1 Different nodes

Chapter 2

Problem Description

2.1 Overview

Kiwi's traveler wants to travel in N different areas in N days, let's denote A the set of areas the traveler wants to visit:

$$A = \{A_1, A_2, \dots, A_N\}$$

where each A_j is a set of airports in area j :

$$A_j = \{a_{j,1}, a_{j,2}, \dots, a_{j,k_j}\}$$

where a_{j,k_j} being airports in area j and k_j is the number of airports in area j .

The traveler has to visit one area per day. He has to leave this area to visit a new area by flying from the airport he flew in. He leaves from a known starting airport and has to do his journey and come back to the starting area, not necessarily the starting airport. There are flight connections between different airports, with different prices depending on the day of the travel: we can write c_{ij}^d the cost to travel from $city_i$ to $city_j$ on day d . We do not necessarily have $c_{ij}^d = c_{ji}^d$ neither $c_{ij}^{d_1} = c_{ij}^{d_2}$ if $d_1 \neq d_2$. The problem can hence be characterised as assymetric and time dependant as discussed in Section 1.2.

The aim of the problem is to find the cheapest route for the traveler's journey.

The problem itself had not been mathematically defined in previous research, and we found it particularly valuable in our study to rigorously formulate the problem mathematically, as it provided a clear framework to analyse and understand its complexities.

We can then formulate the problem as follow:

- $\mathcal{A} = \{1, 2, \dots, N\}$: Set of areas.
- $A_j = \{a_{j,1}, a_{j,2}, \dots, a_{j,k_j}\}$: Set of airports in area $j \in \mathcal{A}$.
- $\mathcal{D} = \{1, 2, \dots, N\}$: Set of days.
- $U_d \subseteq \mathcal{A}$: Set of areas that have not been visited by the end of day d .

Parameters

- c_{ij}^d : Cost to travel from airport i to airport j on day $d \in \mathcal{D}$.

Variables

- x_{ij}^d : Binary variable which is 1 if the traveler flies from airport i to airport j on day d , and 0 otherwise.
- v_j^d : Binary variable which is 1 if area j is visited on day d , and 0 otherwise.

Constraints

1. Starting and Ending Constraints:

- The traveler starts at the known starting airport S_0 .
- The traveler must return to an airport in the starting area on the final day N .

2. Flow Constraints:

- The traveler must leave each area and arrive at the next area on consecutive days, the next area has not been visited yet.
- Ensure that the traveler can only fly into and out of the same airport within an area.

- Ensure each area is visited exactly once.
- Update the unvisited list as areas are visited.

Objective Function

The goal is to minimise the journey's total travel cost:

$$\min \left(\sum_{d=2}^{N-1} \sum_{i \in \bigcup_{k=2}^{N-1} A_k} \sum_{j \in \bigcup_{k=3}^N A_k} c_{ij}^d x_{ij}^d + \sum_{j \in A_1} c_{S_0,j}^1 x_{S_0,j}^1 + \sum_{i \in A_N} \sum_{j \in A_1} c_{ij}^N x_{ij}^N \right)$$

Constraints

- Starting at the known starting airport S_0 at take an existing flight connection:

$$\sum_{j \in A_1} x_{S_0,j}^1 = 1$$

$$\forall d \in \mathcal{D}, c_{S_0,j}^d \in \mathbb{R}^{+*}$$

- Visit exactly one airport in each area each day:

$$\sum_{i \in A_d} \sum_{j \in A_{d+1}} x_{ij}^d = 1 \quad \forall d \in \{1, 2, \dots, N-1\}$$

- Ensure the traveler leaves from the same airport they arrived at the previous day:

$$\sum_{k \in A_d} x_{ik}^d = \sum_{k \in A_{d-1}} x_{ki}^{d-1} \quad \forall i \in \bigcup_{j=1}^N A_j, \forall d \in \{2, 3, \dots, N\}$$

- Return to an airport in the starting area on the final day with an existing flight connection:

$$\sum_{i \in A_N} \sum_{j \in A_1} x_{ij}^N = 1$$

$$\forall (i, j) \in A_N \times A_1, c_{i,j}^N \in \mathbb{R}^{+*}$$

- Ensure each area is visited exactly once:

$$\sum_{d \in \mathcal{D}} v_j^d = 1 \quad \forall j \in \mathcal{A}$$

- Update the unvisited list:

$$v_j^d = 1 \implies j \notin U_d \quad \forall j \in \mathcal{A}, \forall d \in \mathcal{D}$$

- Ensure a flight on day d between i and j exists only if the cost exists and j is in the unvisited areas on day d :

$$x_{ij}^d \leq c_{ij}^d \cdot v_j^d \quad \forall i, j \in \left(\bigcup_{j=1}^N A_j\right)^2, \forall d \in \mathcal{D}$$

$$x_{ij}^d \leq v_j^d \quad \forall j \in \bigcup_{j=1}^N A_j, \forall d \in \mathcal{D}$$

- Binary variable constraints:

$$x_{ij}^d \in \{0, 1\} \quad \forall (i, j) \in \left(\bigcup_{j=1}^N A_j\right)^2, \forall d \in \mathcal{D}$$

$$v_j^d \in \{0, 1\} \quad \forall j \in \mathcal{A}, \forall d \in \mathcal{D}$$

2.2 Instances

2.2.1 Description

We are given a set of 14 Instances $I_n = \{I_1, I_2, \dots, I_{13}, I_{14}\}$ that we have to solve. Every instances has the same overall structure.

For example, the first few lines of I_4 are:

13 GDN
 first
 WRO DL1
 second
 BZG KJ1
 third
 BXP LB1

That means that the Traveller will visit 13 different areas, he starts from airport GDN, that belongs to the starting area. Then we are given the list of airports that are in every zone. For example, the second zone is named second and has two airports: WRO and DL1.

After all the information regarding the areas and the airports we have the flight connections informations. In Table 2.1, few flights are displayed from I_6 for illustrative purpose.

TABLE 2.1: Flight connections sample I6

| Departure from | Arrival | Day | Cost |
|----------------|---------|-----|------|
| KKE | BIL | 1 | 19 |
| UAX | NKE | 73 | 16 |
| UXA | BCT | 0 | 141 |
| UXA | DBD | 0 | 112 |
| UXA | DBD | 0 | 128 |
| UXA | DBD | 0 | 110 |

For every instance I_i , we know what connections exist between two airports for a specific day and the associated cost. There might be in some instances flights connections at day 0, this means these connections exist for every day of the journey at the same price. Furthermore, we could have same flight connections at a specific day but with different prices. We then have to consider only the more relevant connections i.e. the flight connection with the lowest fare, on 2.1 we only consider the flight from UXA to DDB with the associated cost of 110.

2.2.2 General formulation

We decided to formulate the problem mathematically because it was not done in the existing papers, and we found it useful to clearly understand the problem's instances and their characteristics.

An instance I_i can be mathematically defined as follows:

$$I_i = (N_i, S_{i0}, A_i, F_i)$$

where:

- **Number of Areas N_i :**

$$N_i \in \mathbb{N}$$

The total number of distinct areas in instance I_i .

- **Starting Airport S_{i0} :**

$$S_{i0} \in \text{Airports}$$

The starting airport of the traveller.

- **Airports in Each Area:**

$$A_i = \{A_{i,1}, A_{i,2}, \dots, A_{i,N_i}\}$$

where each $A_{i,j}$ is a set of airports in area j for instance i :

$$A_{i,j} = \{a_{i,j,1}, a_{i,j,2}, \dots, a_{i,j,k_j}\}$$

with a_{i,j,k_j} being airports in area j and k_j is the number of airports in area j .

- **Flight Connections:**

$$F_i = \{F_{i,0}, F_{i,1}, F_{i,2}, \dots, F_{i,N_i}\}$$

where each flight matrix $F_{i,k}$ represents the flight information of instance i on day k :

$$F_{i,k} = \begin{pmatrix} a_{i,k,1}^d & a_{i,k,1}^a & f_{i,k,1} \\ a_{i,k,2}^d & a_{i,k,2}^a & f_{i,k,2} \\ \vdots & \vdots & \vdots \\ a_{i,k,l_{k,i}}^d & a_{i,k,l_{k,i}}^a & f_{i,k,l_{k,i}} \end{pmatrix}$$

– **Columns:**

- * Departure Airport: $a_{i,k,j}^d$ (Departure airport for the j -th flight on day k)
- * Arrival Airport: $a_{i,k,j}^a$ (Arrival airport for the j -th flight on day k)
- * Cost: $f_{i,k,j}$ (Cost of the j -th flight on day k), where $j \in [1, l_{k,i}]$

– **Rows:** Each row corresponds to a specific flight on day k . The number of rows $l_{k,i}$ depends on the number of flights available on that day.

2.2.3 Kiwi's rules

When solving all the instances, Kiwi's defined time limits constraints based on the nature of the instance. We can summarise these constraints in the Table above:

TABLE 2.2: Time limits based on the number of areas and airports

| Instance | nb areas | Nb Airports | Time limit (s) |
|----------|------------|-------------|----------------|
| Small | ≤ 20 | < 50 | 3 |
| Medium | ≤ 100 | < 200 | 5 |
| Large | > 100 | | 15 |

All the useful information about the instances such as the starting airport, the associated area, the range of airports per area, the number of airports and the time limit constraints are defined in Table 2.3.

TABLE 2.3: Instances and their respective parameters

| Instances | Starting Area - Airport | N° areas | Min - Max airport per area | N° Airports | Time Limit (s) |
|-----------|----------------------------|-------------|-------------------------------|----------------|-------------------|
| I1 | Zona_0 - AB0 | 10 | 1 - 1 | 10 | 3 |
| I2 | Area_0 - EBJ | 10 | 1 - 2 | 15 | 3 |
| I3 | ninth - GDN | 13 | 1 - 6 | 38 | 3 |
| I4 | Poland - GDN | 40 | 1 - 5 | 99 | 5 |
| I5 | zone0 - RCF | 46 | 3 - 3 | 138 | 5 |
| I6 | zone0 - VHK | 96 | 2 - 2 | 192 | 5 |
| I7 | abfuidmorz - AHG | 150 | 1 - 6 | 300 | 15 |
| I8 | atrdrwkbz - AEW | 200 | 1 - 4 | 300 | 15 |
| I9 | fcjsqtmccq - GVT | 250 | 1 - 1 | 250 | 15 |
| I10 | eqlfrvhlwu - ECB | 300 | 1 - 1 | 300 | 15 |
| I11 | pbggaejrjv - LIJ | 150 | 1 - 4 | 200 | 15 |
| I12 | unnwaxhnoq - PJE | 200 | 1 - 4 | 250 | 15 |
| I13 | hpkogdfpf - GKU | 250 | 1 - 3 | 275 | 15 |
| I14 | jjewssxvsc - IXG | 300 | 1 - 1 | 300 | 15 |

Chapter 3

Methodology

(TODO) Describe implementation details

3.1 Monte Carlo Tree Search implementation

3.1.1 General flow

Based on the discussion in Chapter 1, the flow of the Monte Carlo Tree Search algorithm is summarised in Figure 3.1:

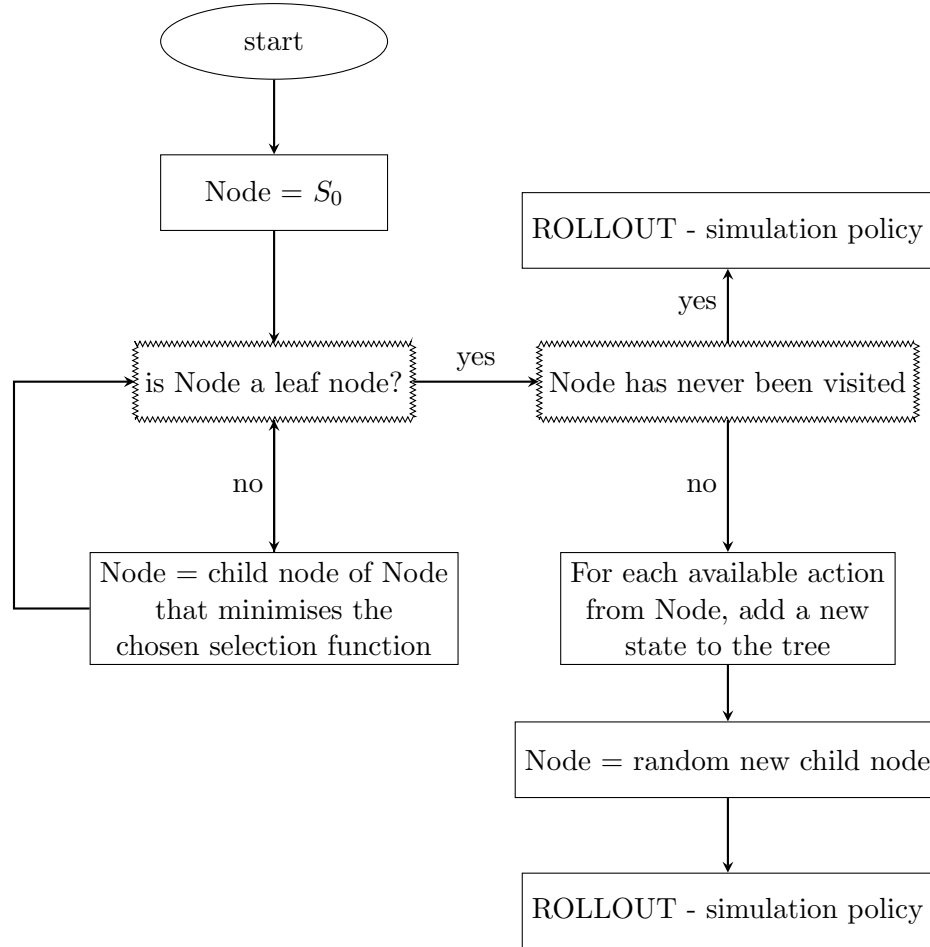


FIGURE 3.1: Flow MCTS

For every iteration of this algorithm - there are four different phases:

1. **Selection:** Starting from the root node (the starting airport S_{i0} for I_i), select successive child nodes (airports that are in unvisited areas) until a leaf node (the airport in the initial area - not necessarily the starting airport) is reached. Use the chosen Selection function to evaluate which node's is the most promising. In the illustrative example in Section ??, we used the UCB1 function for the selection

function. We were also dealing with a maximisation problem, hence we selected nodes with the highest UCB1 value. A contrario, in Kiwi's minimisation problem, nodes are evaluated based on the lowest value of the selection function.

2. **Expansion:** If the selected node is not a terminal node, expand the tree by adding all possible child nodes.
3. **Simulation:** From the newly added node, perform a simulation (based on the simulation policy) until we reach a terminal node i.e we find a feasible solution.
4. **Backpropagation:** Update the values of the nodes along the path from the newly added node to the root based on the result of the simulation.

$$\mathcal{B}(S_i^{n_i, t_i}) = S_i^{n_i+1, t_i} + \mathcal{R}(S_i^{n_i, t_i}) \quad (3.1)$$

where $\mathcal{R}(S_i^{n_i, t_i})$ is the cost of the solution found after performing a simulation from node $S_i^{n_i, t_i}$.

3.1.1.1 Data Preprocessing

In order to implement our MCTS' solution, the first thing to implement was a `data_preprocessing` class in order to preprocess the given instance. Kiwi's challenge has been solved using Python 3.10 on VS Code 1.92.2. Our Python code is structured using object-oriented programming. This `data_preprocessing` class is represented on Figure 3.2. The input is an instance I_i , as defined in Chapter 2:

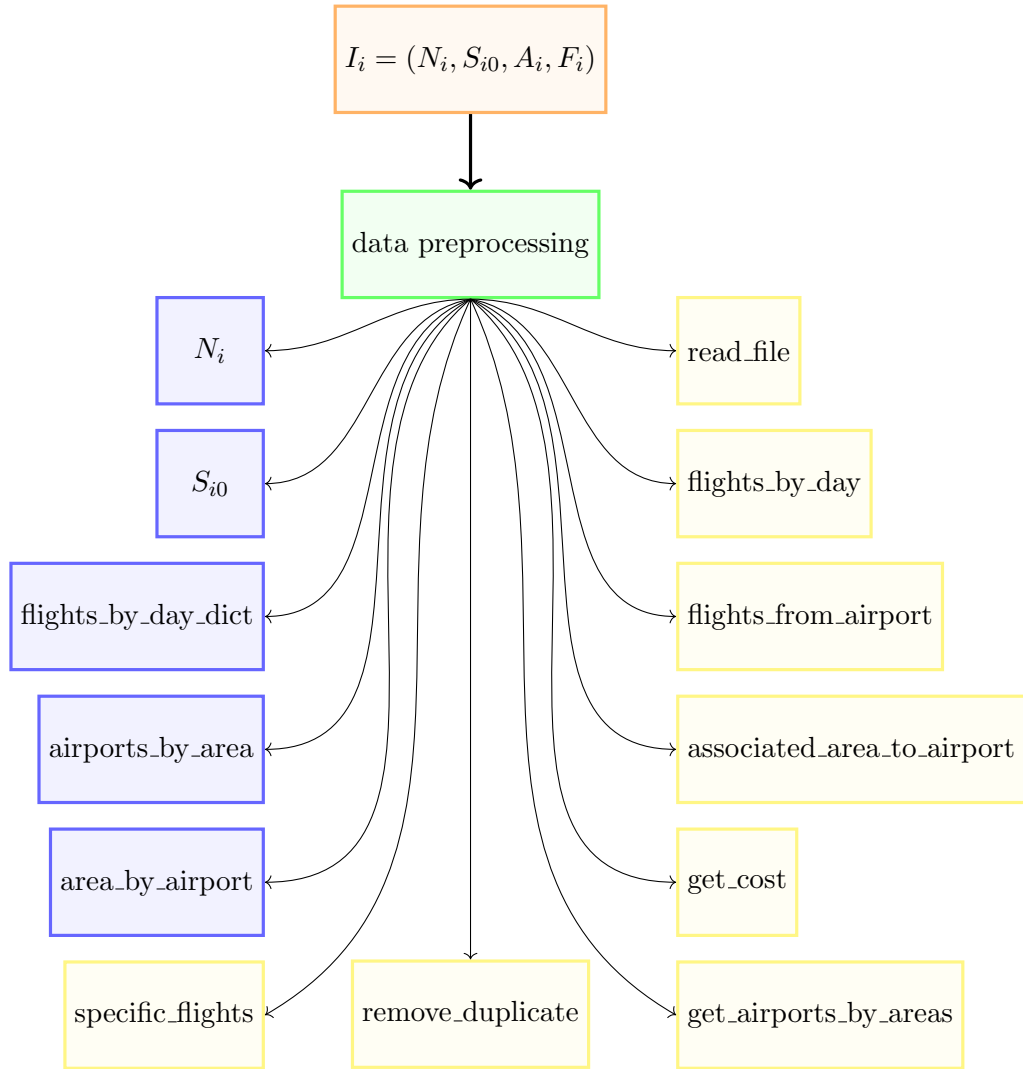


FIGURE 3.2: Explanation of the data preprocessing class

Different useful methods are implemented within the `data_preprocessing` class to compute and manage various attributes required for the problem at hand. These methods are designed to prepare and structure the data, making it easier to use in subsequent phases

of the algorithm. For example, the `remove_duplicate` method ensures that only the cheapest flight connections are considered between two airports if multiple flight connections exist at different prices on the same day. Other methods, such as `flights_by_day_dict` and `get_airports_by_areas` organise the data. The first method regroup all the flights by their respective days, creating a dictionary where each key represents a day and its corresponding value is a list of available flights. The second is regrouping all the airports present in the different areas. Finally, others methods like `specific_flights` will be helpful in the algorithm's development gives all the possible flight connections from a specific airport on a specific day considering the `visited_areas`, it hence gives you all the possibles actions from a node.

Given that Python is relatively slower in terms of computation compared to other programming languages, we opted to use as much as possible dictionaries. Dictionaries allow for efficient data retrieval based on a key, with an average time complexity of $\mathcal{O}(1)$. This choice enhances the performance of the data preprocessing step, ensuring that the algorithm runs more efficiently despite Python's inherent limitations.

3.1.1.2 Node

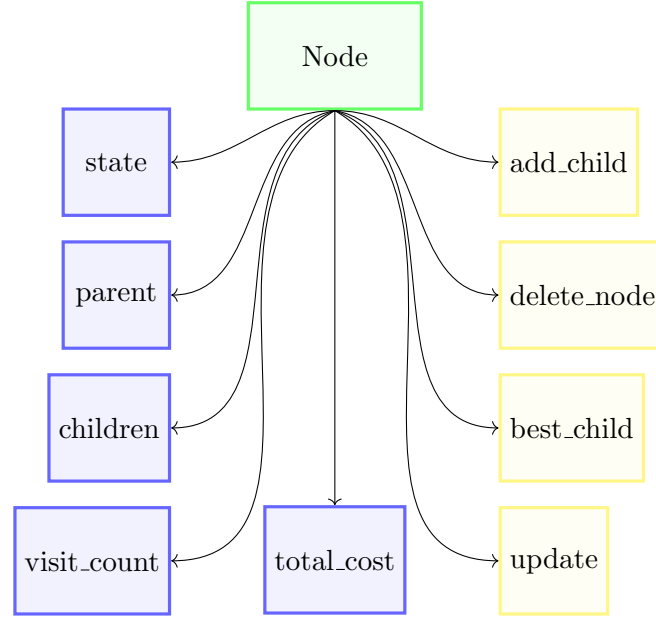


FIGURE 3.3: Explanation of the Node class

As mentioned earlier in Section 1.3.2, we use a Node structure in our algorithm, hence we implemented a Node class. Each Node has a reference to a parent node (unless it is the root node) and may have one or more child nodes (unless it is a leaf node). These relationships form a tree structure where each node can expand into potential future states, guiding the search process. The `visit_count` tracks the number of times a node has been visited during the MCTS process. This is crucial for evaluating the node's importance and for calculating score of the node with the selection function. The `state` is a dictionary that contains node's current information:

- `current_airport`: The airport where the traveler is at this node.
- `current_day`: The day of the trip at this node.
- `remaining_zones`: The zones that still need to be visited to complete the journey.
- `visited_zones`: The zones that have already been visited to ensure that all zones are visited exactly once during the trip.
- `total_cost`: It represents the accumulated cost of the current solution path leading to this node.

Additionally, to manage the expansion of child nodes, the `add_child` method is defined. This method generates new nodes based on the possible actions available from the current node, the potential flight connections from the current airport on this specific day, given the current path taken so far. These new nodes represent the next possible states in the traveler's journey, allowing the search tree to expand and explore different travel routes. Finally, the `delete_node` method can be used to delete a node from the list of its parent's children.

3.2 The different policies

In the previous section, we outlined the general flow of the MCTS algorithm, focusing on two core classes, `data_preprocessing` and `Node`, that are central in MCTS' implementation.

In Section 1.4, we explored the various selection policies that guide the decision-making process within MCTS. Although there is a limited literature review, we decided to parameterise not only the selection policy but also the simulation and expansion policy.

3.2.1 Simulation policies

When you simulate from a given node in the tree, the goal is to find a feasible combination of airports that could be a solution to our problem. Then from this current node, you have the current state (defined in Section 3.1.1.2), so you have to choose for the remaining actions based on the simulation policy.

We decided to define three distinct simulation policies:

- **Random policy:** This policy selects a random action from the set of available actions, introducing variability and exploration in the simulation process.
- **Greedy Policy:** This policy selects the action that corresponds to the cheapest available flight connection, thus prioritising cost minimisation at each step.
- **Tolerance Policy (with coefficient c):** This policy selects an action randomly from a subset of actions that are within a certain tolerance level of the minimum cost action. The tolerance level is defined by a coefficient c , allowing for a balance between exploration and exploitation.

The tolerance heuristic is defined as follows:

- Identify the cheapest flight connection among the available actions c_{min} .
- Filter the actions to include only those with a cost less or equal than $c_{min}(1 + c)$.
- Randomly select an action from this filtered set.

3.2.2 Expansion policies

When expanding a node, it's theoretically possible to expand all available child nodes i.e. add all the possible flight connections from a node at a specific day to the tree. However, in practice, this can be computationally expensive and time-consuming, particularly in problems with a large number of possible actions. To address this, heuristic approaches often involve compromises that enhance the efficiency of the search process by selectively expanding certain nodes rather than all possible ones.

In our implementation we defined two expansion policies:

- **Top-K Actions Policy:** This policy expands the nodes corresponding to the cheapest flight connections available. Specifically, it sorts all possible actions based on their associated costs and selects the top k actions with the lowest costs, where k is regulated by a parameter called `number_of_children`. This approach ensures that only the most promising actions, in terms of cost efficiency, are considered during expansion. This policy narrow down the search space but can reach to local optima.
- **Ratio Best-Random Policy:** This policy takes a more balanced approach by combining the selection of the best actions with a degree of randomness. First, it calculates the number of top actions to select based on a predefined ratio, c , of `number_of_children`. The top actions are chosen based on their costs, similar to the Top-K Actions Policy. After selecting these best actions, the policy randomly selects additional actions from the remaining pool to reach the desired number of children. This policy is designed to explore a broader range of possibilities while still prioritising cost-effective options.

In addition to these policies, as already mention, the parameter `number_of_children` plays a critical role in regulating the maximum number of children that can be expanded

from any given node. This limitation controls the size of the search tree, especially in larger instances where again, expanding too many nodes could make the algorithm computationally exhaustive.

3.2.3 MCTS' Pseudo-code

In this section, we go into more detail about how we implemented the algorithm in practice by examining the different functions of our MCTS class. The main idea is:

Algorithm 1 Monte_Carlo_Tree_Search

```

1: Initialise Root_Node with Initial_State
2: while Tree is not fully explored do
3:    $Node \leftarrow \text{Select}(Root\_Node)$ 
4:   if  $Node$  is not fully expanded then
5:      $Node \leftarrow \text{Expand}(Node)$ 
6:   end if
7:    $Cost \leftarrow \text{Simulate}(Node)$ 
8:    $\text{Backpropagate}(Node, Cost)$ 
9: end while
10: return  $Best\_Leaf\_Node$ 

```

The **Select** function returns two arguments: a boolean and a node. The boolean indicates to the expansion function whether expansion is necessary (True means no expansion needed, False means yes):

Algorithm 2 Select_Function

```

1: Input: Node
2: Current  $\leftarrow$  Node
3: while Current.Children is not empty do
4:   if Current is not fully expanded then
5:     UnvisitedChildren  $\leftarrow$  Children with VisitCount = 0
6:     if UnvisitedChildren is not empty then
7:       SelectedChild  $\leftarrow$  Randomly select from UnvisitedChildren
8:       return True, SelectedChild
9:     end if
10:  else
11:    Current  $\leftarrow$  BestChild(Current)
12:  end if
13: end while
14: if Current.Children is empty and Current.State["current_day"] ==  $N_{Areas}$  then
15:  return False, Current
16: else if Current.Children is empty and Current.State["current_day"] ==  $N_{Areas}$ 
    then
17:  return False, Current
18: else if Current.State["current_day"] ==  $N_{Areas} + 1$  then
19:  return True, Current
20: end if

```

We backpropagate the node using the update method of the node. The new node becomes the parent of this node, and we do that until *Node* is *None*, i.e., we have backpropagated all the information up to the root node.

Algorithm 3 Backpropagate_Function

```

1: while Node is not None do
2:   Node.Update(Cost)
3:   Node  $\leftarrow$  Node.Parent
4: end while

```

The transition function modifies the states of a node by updating the current airport, the visited zones, remaining zones, etc.

Algorithm 4 Transition Function

```

1:  $New\_State \leftarrow \text{Copy of } State$ 
2:  $New\_State.Current\_Day \leftarrow State.Current\_Day + 1$ 
3:  $New\_State.Current\_Airport \leftarrow Action[0]$ 
4:  $New\_State.Total\_Cost \leftarrow State.Total\_Cost + Action[1]$ 
5:  $Update(New\_State.Path, New\_State.Current\_Airport)$ 
6:  $Remove\_Visited(New\_State.Remaining\_Zones, New\_State.Current\_Airport)$ 
7:  $Add\_Visited(New\_State.Visited\_Zones, New\_State.Current\_Airport)$ 
8: return  $New\_State$ 

```

Finally, the Best Child function, defined in the Node class is based on the selection function UCB, UCB1-Tuned, SP and Bayesian, computes the score of the visited nodes and pick the one that minimises the selection function.

Algorithm 5 Best Child

Require: *Selection_Function*

```

1:  $Visited\_Children \leftarrow \text{Children with } visitCount > 0$ 
2:  $Choices\_Weights \leftarrow [Selection\_Function(child) \text{ for } child \text{ in } Visited\_Children]$ 
3:  $Best\_Child\_Node \leftarrow \text{Child with minimum } Choices\_Weights$ 
4: return  $Best\_Child\_Node$ 

```

Chapter 4

Results and performance

(TODO) Present the results and discuss any differences between the findings and your initial predictions/hypothesis

(TODO) Interpret your experimental results - do not just present lots of data and expect the reader to understand it. Evaluate what you have achieved against the aims and objectives you outlined in the introduction

4.1 Hypothesis

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