

# From Parameter Tuning to Dynamic Heuristic Selection

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Course: Distributed Systems Engineering

Matriculation number: 4733680

Matriculation year: 2017

## Master Thesis

to achieve the academic degree

## Master of Science (M.Sc.)

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Submitted on: 11th May 2020

## Aufgabenstellung für die Masterarbeit

Name, Vorname: Semendiak, Yevhenii

Studiengang: Master DSE

Matr. Nr.: 4 7 3 3 6 8 0

Thema:

From Parameter Tuning to Dynamic Heuristic Selection

Zielstellung :

Metaheuristic-based solvers are widely used in solving combinatorial optimization problems. A choice of an underlying metaheuristic is crucial to achieve high quality of the solution and performance. A combination of several metaheuristics in a single hybrid heuristic proved to be a successful design decision. State-of-the-art hybridization approaches consider it as a design time problem, whilst leaving a choice of an optimal heuristics combination and its parameter settings to parameter tuning approaches. The goal of this thesis is to extend a software product line for parameter tuning with dynamic heuristic selection; thus, allowing to adapt heuristics at runtime. The research objective is to investigate whether dynamic selection of an optimization heuristic can positively effect performance and scalability of a metaheuristic-based solver.

For this thesis, the following tasks have to be fulfilled:

- Literature analysis covering closely related work.
- Development of a strategy for online heuristic selection.
- Implementation of the developed strategy.
- Evaluation of the developed approach based on a synthetic benchmark.
- (Optional) Evaluation of the developed approach with a problem of software variant selection and hardware resource allocation.

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Institut: Software- und Multimediatechnik

Beginn am : 01.10.2019

Einzureichen am : 09.03.2020



Unterschrift des verantwortlichen Hochschullehrers

## Abstract

The importance of balance between exploration and exploitation plays a crucial role while solving combinatorial optimization problems. This balance is reached by two general techniques: by using an appropriate problem solver and by setting its proper parameters. Both problems were widely studied in the past and the research process continues up until now. The latest studies in the field of automated machine learning propose merging both problems, solving them at design time and later strengthening the results at runtime. To the best of our knowledge, the *generalized* approach for solving the parameter setting problem in heuristic solvers has not yet been proposed. Therefore, the concept of merging heuristic selection and parameter control has not been introduced.

In this thesis we propose an approach for generic parameter control in meta-heuristics by means of reinforcement learning (RL). Making a step further, we suggest a technique for merging the heuristic selection and parameter control problems and solving them at runtime using RL-based hyper-heuristic. The evaluation of the proposed parameter control technique on a symmetric traveling salesman problem (TSP) revealed its applicability by reaching the performance of tuned in offline and used in isolation underlying meta-heuristic. Our approach provides the results on par with the best underlying heuristics with tuned parameters.





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# 1 Introduction

## 1.1 Motivation

Heuristic-based optimization is a popular research area. Various optimization problems (OPs) are defined and can be tackled by heuristic algorithms [14, 43, 63]. Unfortunately, an ideal algorithm that can solve every OP does not and cannot exist. This issue was formalized by the *no-free-lunch theorem for optimization* (NFLT) [121], which states that “all search algorithms have the same average performance over all possible optimization problems”. Heuristic solver acts by means of *exploration* (effort diversification over a search space) and *exploitation* (effort intensification in a promising area) operations. The success of heuristic on the problem at hand is defined by the exposed strength of both operations (E&E) and the provided balance between them (EvE). Both E&E and EvE characteristics can be controlled in several ways.

Firstly, one could try to set proper values of hyper-parameters exposed by the algorithm. This process is formalized under the notion of *parameter settings problem* (PSP), whose resolution can be done before running the algorithm (design time), or while it solves the OP (runtime). The former approach is also called *parameter tuning* and can be tackled by numerous universal tuning systems [41, 58, 59, 79, 93]. A key assumption of this software is an expensive evaluation of the target system in terms of computational resources. High expensiveness is tackled by a surrogate learning model creation, which is then used to simulate the direct evaluations. The latter approach called *parameter control* was originally introduced for evolutionary algorithms [66] and nowadays appears in an *algorithm-dependent* manner. However, even a proper parameter setting may not lead to the best results for the problem at hand.

Secondly, one could try to select a proper algorithm. It was formalized as the *algorithm selection problem* (ASP) and defined as a process of searching for an appropriate solver for the problem at hand. ASP resolves the direct consequence of NFLT, which states that a single algorithm cannot be used to tackle various problems. Hyper-heuristics are commonly used for solving ASPs. They may perform low-level heuristic selection before solving [22] the actual problem, or at runtime [22]. To operate online, hyper-heuristics often utilize reinforcement learning (RL) techniques [84, 86], while for design time, a regular parameter tuning could be used.

The research has not been standing at a standstill and nowadays the researchers are actively attempting to merge ASP and PSP into a united *algorithm selection and parameter setting problem* (APSP). For instance, in automatic machine learning such combination was formalized as the *combined algorithm selection and hyper-parameter optimization* problem (CASH) [112], while for heuristics the explicit studies of APSP merging and solving at runtime were not found. To tackle ML CASH problem several frameworks based on the existing parameter tuning systems were created [44, 88, 112]. However, those solutions are not applicable in case of heuristics, since they are (1) purely related to ML field and (2) acting at design time due to ML techniques nature. One may follow the ML approach of the united APSP search space definition and solving for heuristics, but it is applicable *only* at design time. Nevertheless, when it comes to runtime, it turns out that the universal technique for setting the parameters online (parameter control) in heuristics has not yet been proposed. It is essential, since the generic approach to tackle PSP is one of two required methodologies for solving heuristic APSP at runtime. The other building block (ASP) is already available in online hyper-heuristics.

### 1.2 Research objective

The goal of this thesis is to improve the quality of online heuristic-based optimization. The research objective is to determine whether it is possible to solve both PSP and ASP, while solving the OP. In order to reach our objective we need to answer the following research questions:

- **RQ1** Is it possible to perform the algorithm configuration at runtime on a generic level?
- **RQ2** Is it possible to simultaneously perform algorithm selection and parameters adaptation while solving an OP?
- **RQ3** What is the effect of selecting and adapting algorithms while solving an OP?

### 1.3 Solution overview

In this thesis we propose the unification of both ASP and PSP into a single problem. To do so, we firstly introduce a generic runtime PSP solution; secondly, we suggest joining several PSPs search spaces into a united APSP. The consequence of merging several PSPs into a single APSP is the appearance of *sparse* search spaces, where the percentage of properly defined configurations is low due to requiring and prohibiting dependencies among parameters (e.g., each algorithm has its own required set of parameters).

To overcome the sparseness issue we propose a complex solution, which is spread in both search space structure and sampling process. For the APSP representation we suggest using a data structure, similar to feature trees from software product lines field. By doing so, we treat a solver type and its hyper-parameters uniformly. The dependencies between parameters are explicitly handled in the form of parent-child relationship. As a result, the search space could be viewed as a layered structure, where on the first level the algorithm type is defined, and on the level(s) below its respective hyper-parameters are specified. The prediction process is made sequentially for each level, utilizing the available performance evidence in a form of already tried configurations and respective improvements. Therefore, in the united APSP we firstly build a surrogate model for the algorithm type prediction. Afterwards, when the solver type is selected, we filter the performance evidence to operate on data, which is relevant to the selected algorithm type. With this filtered data we build a surrogate for the second level and predict the parameters values on second level. This level-wise process continues until obtaining a completed configuration. Next, we continue solving the underlying OP with the defined algorithm type and the predicted configuration to obtain new evidence and repeat configuration prediction process. This reinforcement learning technique enables us to solve the APSP online, while iteratively tackling the OP at hand. The proposed concept evaluation showed that: (1) applying the generic parameter control to each among the reviewed meta-heuristics results in the solution quality, comparable and in some cases even outperforming the quality of tuned in offline parameters; (2) our APSP tackling approach is preferable in cases, when the heuristics dominance and their parameters are unknown beforehand.

The structure of this thesis is organized as follows. Firstly, in Chapter 2 we refresh the readers' background knowledge in the field of optimization problems and solver types, focusing on heuristics. We also review the parameter setting and the available solutions for this problem. In Chapter 3 one will find a description of the proposed approach for generic parameter control and APSP problem unification. There we also present both structural and functional requirements for system components. Chapter 4 is dedicated to the review of implementation details, including a code basis selection, the aforementioned requirements realization and the developed system workflow representation. We evaluate the proposed concept and discuss the results in Chapter 5. Chapter 6 concludes the thesis and Chapter 7 describes the future work.

## 2 Background and Related Work Analysis

In this Chapter we provide the reader with a review of the basic knowledge in fields of optimization problems and approaches for solving them. A reader, experienced in field of optimization and search problems, may consider this chapter as an obvious discussion of well-known facts. If such notions as a *parameter tuning* and a *parameter control* are not familiar to you or seem the same, we highly encourage you to spend some time reading this chapter carefully. In any case, it is worth for everyone to refresh the knowledge with a coarse-grained description of topics, mentioned in this section and examine the examples of hyper-heuristics in Section 2.2.5 and systems for parameter tuning in Section 2.3.2.

The structure of this Chapter is defined as follows. Firstly, we give an informal definition of an optimization problem and enumerate possible solver types in Section 2.1. Secondly, we pay attention to the heuristic solvers, their weak points and *No Free Lunch Theorem* in Section 2.2. Afterwards, in Section 2.3 we discuss the influence of parameter setting and possible approaches to set the parameters. Section 2.4, dedicated to *Combined Algorithm Selection and Hyper-parameter Tuning* problem, is followed by conclusion on the literature analysis outlining the thesis' scope in Section 2.5.

### 2.1 Optimization Problems and their Solvers

Our life is full of different difficult and sometimes contradicting choices. Optimization is an art of making good decisions.

A decision between working hard or going home earlier, to buy cheaper goods or to follow brands, to isolate ourselves or to visit friends during the quarantine, to spend more time on a trip planning or to start it instantly. Each decision that we make, has its consequences.

Figure 2.1 outlines the trade-off between decision quality and an amount of effort spent. The underlying idea of the research in optimization is to squash this curve simultaneously down and to the left, therefore, deriving a better result with less cost when solving the optimization problem.

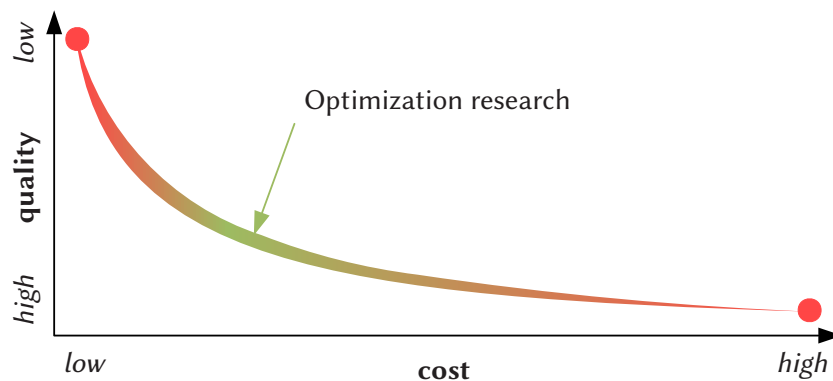


Figure 2.1 Optimization trade-off.

### 2.1.1 Optimization Problems

While the *search problem* (SP) defines the process of finding a possible solution for the *computation problem*, the *optimization problem* (OP) defined as a special case of the SP, focused on the process of finding the *best possible* solution for computation problem [51].

The focus of this thesis is the optimization problems.

Most studies conducted in this field have tried to formalize the OP concept, but the underlying notion is so vast that it is hard to exclude the application domain from the definition. The description of every possible optimization problem and all approaches to its solving are not in the scope of this thesis, while we consider it necessary to present a coarse-grained review in order to make sure that readers are familiar with all the terms and notions mentioned in the thesis.

To begin with, let us define the optimization *subject*. Analytically, it could be represented as the function  $Y = f(X)$  that accepts some input  $X$  and reacts to it, providing an output  $Y$ . Informally, it could be imagined as the *target system*  $f$  (TS), shown in Figure 2.2. It accepts the input information with its *inputs*  $X_n$ , which are sometimes called variables or parameters, processes them performing some *task* and produces the result on its *outputs*  $Y_m$ .

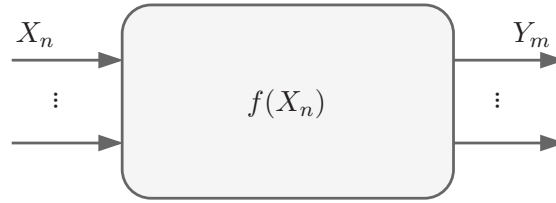


Figure 2.2 Optimization Target System.

Each (unique) pair of sets  $X_n^i$  and respective  $Y_m^i$  form the *Solution*<sup>*i*</sup> for computational problem. All possible inputs  $X^i$ , where  $i = 1 \dots N$  form the *search space* of  $N$  size, while all outcomes  $Y^i$ , where  $i = 1 \dots M$  form an *objective space* of  $M$  size.

The solution is characterized by the *objective value(s)* – a quantitative measure of TS performance that we want to minimize or maximize in the optimization problems. We could obtain those value(s) directly, by reading the output on  $Y_m$ , or indirectly, for instance, noting the wall clock time TS took to produce the output  $Y^i$  for given  $X^i$ . The solution objective value(s) form the *object* of optimization. For the sake of simplicity we here use  $Y_m$ , *outputs* or *objectives* interchangeably as well as  $X_n$ , *variables* or *parameters*.

Next, let us highlight the target system characteristics. In works [2, 14, 32, 46] dedicated to solving the OPs, the authors distinguished OP characteristics that overlap through each of these works. Among them, we found the following properties to be the most important ones:

- **Input data type** of  $X_m$  is a crucial characteristic. All input variables could be (1) *discrete*, where representatives are binary strings, integer-ordered, or categorical data, (2) *continuous*, where variables are usually a range of real numbers, or (3) *mixed*, as the mixture of the previous two cases.
- **Constraints** describe the relationships among inputs and explain the dependencies in allowable values for them. As an example, imagine that having  $X_n$  equal to *value* implies that  $X_{n+k}$  should not appear at all, or could take only some subset of all possible values.
- **Type of target system** is an amount of exposed knowledge about the dependencies  $X \rightarrow Y$  before the optimization process starts. Taking this into consideration, an optimization could be



of several types: *white-box* — it is possible to derive the algebraic model of TS, *gray-box* — the amount of exposed knowledge is significant but not enough to build the algebraic model and *black-box* — the exposed knowledge is mostly negligible.

- **Determinism of TS** is one of the possible challenges, when the output is uncertain. TS is *deterministic*, when in each time it provides an equal output for the same input. However, in most real-life challenges engineers tackle *stochastic* systems, the output of which is affected by random processes happened inside TS.
- **Cost of evaluation** is an amount of resources (energy, time, money, etc.) TS should spend to produce the output for particular input. It varies from *cheap*, when TS could be an algebraic formula and task evaluation is a simple mathematic computation, to *expensive*, when the TS is a pharmaceutical company, and the task is to perform a whole bunch of tests for a new drug, which may last years.
- **Number of objectives** is a size of the output vector  $Y_m^i$ . With regard to this, the optimization could be either single- ( $m = 1$ ), or multi- ( $m = 2 \dots M$ ) objective, where the result is one single solution, or a set of non-dominated (Pareto-optimal) solutions.

Most optimization problem types could be obtained by combining different types of each characteristic listed above.

In this thesis we tackle practical combinatorial problems, where the most prominent examples are *bin packing* [82], *job-shop scheduling* [17] or *vehicle routing* [113] optimization problems. All combinatorial problems are *NP-Complete* meaning they are in both *NP* and *NP-Hard* complexity classes [48]. NP complexity implies that the solution is verifiable in the polynomial time, while in the NP-Hard case the problem can be transformed into other NP-Complete problem in polynomial time, allowing to use a different solving algorithm.

As an example, let us grasp these characteristics for *traveling salesman problem* (TSP) [3] — an instance of the vehicle routing problem [73] and one of the most frequently studied a combinatorial OP (here we consider deterministic and symmetric TSP). The informal definition of TSP is as follows: “Given a set of  $N$  cities and the distances between each of them, what is the shortest path that visits each city once and returns to the origin city?” With respect to our previous definition of the optimization problem, the target system here is a function that evaluates the length of proposed path. The TSP distance (or cost) matrix is used in this function for the evaluation and it is clear that this TS exposes all internal knowledge therefore, it is a white box. The input  $X_n$  is a vector of city indexes as a result, the type of input data is non-negative integers. There are two constraints for the path: it should contain only unique indexes (visit each city only once) and it should start and end from the same city:  $[2 \rightarrow 1 \rightarrow \dots \rightarrow 2]$ . Since the cost matrix is fixed and not changing during the solving process, the TS is considered to be deterministic and costs of two identical paths are always the same. Nevertheless, there exist Dynamic TSP where the cost matrix changes at runtime to reflect more realistic real-time traffic updates [27]. It is cheap to compute a cost for a given path using the cost matrix therefore, overall solution evaluation in this OP is cheap, and  $n = N!$  is the overall number of solutions. Since we are optimizing only the route distance, this is a single-objective OP.

### 2.1.2 Optimization Problem Solvers

Most of the optimization problems could be solved by an *exhaustive search* — trying all possible combinations of the input variables and choosing the one, which provides the best objective value. This approach guarantees to find a globally optimal solution of the OP. But when the search space size

significantly increases, the brute-force approach becomes infeasible and in many cases solving even the relatively small problem instances take too much time.

Here, different optimization techniques come into play. Characteristics exposed by target system could restrict and sometimes strictly define the applicable approach. For instance, imagine you have a white-box deterministic TS with a discrete constrained input data and cheap evaluation. The OP in this case could be solved using the *Integer Linear Programming* (ILP), or a heuristic approaches. But if this TS turned out to be a black-box, the ILP approaches will not be applicable anymore and one should consider using the heuristics [14].

Evidently, there exist a lot of different facets for optimization problem solvers classification, but they are a subject of many surveying works [14, 43, 63]. In this thesis, as the point of interest we highlight only two of them.

- **Solution quality** perspective:
  1. **Exact** solvers are those algorithms that always provide an optimal OP solution.
  2. **Approximate** solvers produce a sub-optimal output with guarantee in quality (some order of distance to the optimal solution).
  3. **Heuristics** solvers do not give any worst-case guarantee for the final result quality.
- **Solution availability** perspective:
  1. **Completion** algorithms report the results only at the end of their run.
  2. **Anytime** algorithms are designed for stepwise solution improvement thus, could expose intermediate results.

Each of these algorithm characteristics provides their own advantages, having, however, their own disadvantages. For instance, if solution is not available at any time, one will not be able to control the optimization process. On the contrary, if it is available, the overall performance may decrease. If the latter features are more or less self-explanatory, the former require more detailed explanation.

### Solution Quality

**Exact Solvers.** As was stated above, the exact algorithms are those, which always solve OP to guaranteed optimality. For some OP it is possible to develop an effective algorithm that is much faster than the exhaustive search — they run in a super-polynomial time, instead of exponential, still providing an optimal solution. As authors claimed in [120], if the common belief  $P \neq NP$  is true, the super-polynomial time algorithms are the best we can hope to get when dealing with the NP-complete combinatorial problems.

According to the definition in [47], the objective of an exact algorithm is to perform much better (in terms of running time) than the exhaustive search. In both works [47, 120] the authors enumerated main techniques for designing the exact algorithms. Each of these techniques contributes to this ‘better’ independently and later they could be combined.

You may find a brief explanation of them below:

- **Branching and bounding** techniques, when applied to the original problem, split the search space of all possible solutions (e.g. exhaustive enumeration) to a set of smaller sub-spaces. More formally, this process is called *branching the search tree into sub-trees*. This is done with an intent to prove that some of sub-spaces never lead to an optimal solution and thus could be rejected.

- **Dynamic programming across sub-sets** technique could be combined with the branching techniques. After forming the sub-trees, the dynamic programming attempts to derive the solutions for the smaller subsets and later combine them into the solutions for the larger subsets. This process repeats until the solution for original search space obtained.
- **Problem preprocessing** could be applied as an initial phase of the solving process. This technique is dependable upon the underlying OP, but when applied properly, it significantly reduces the running time. A simple example from [120] elegantly illustrates this technique: imagine a problem of finding a pair of two integers  $x_i$  and  $y_i$  in  $X_k$  and  $Y_k$  sets of unique numbers ( $k$  here denotes the size of sets) that sum up to an integer  $S$ . The exhaustive search approach implies enumerating all  $x - y$  pairs. The time complexity in this case is  $O(k^2)$ . But if at first we consider the data preprocessing by sorting and afterwards, using the bisection search repeatedly in these sorted arrays to find  $k$  values  $S - y_i$ , then the overall time complexity reduces to  $O(k \log(k))$ .

**Approximate Solvers.** When the OP cannot be solved to optimal in polynomial time, the only solution is to start thinking of the alternative ways to tackle it. A common decision is to apply the requirement *relaxation techniques* [100] to derive the approximated solution. Approximate algorithms are representatives of the theoretical computer science. They were created in order to tackle the computationally difficult (not solvable in super-polynomial time) white-box OP. Words of Garey and Johnson (computer scientists, authors of *Computers and Intractability* book [48]) could pay a perfect description of such approaches: “I can’t find an efficient algorithm, but neither can all of these famous people.”

Unlike exact, approximate algorithms relax the quality requirements and solve the OP effectively with the provable assurances on the result distance from an optimal solution [119]. The worst-case results quality guarantee is crucial in the approximation algorithms design and involves the mathematical proofs.

How do these algorithms guarantee on quality, if the optimal solution is unknown beforehand? — a reasonable question arises at this point. Certainly, it sounds contradictory, but the comprehensive answer to this question requires an explanation of the key approximation algorithms design techniques that is not in the scope of this thesis. Nevertheless, let us briefly describe these techniques.

In [119] the authors provided several techniques to approximate solvers’ design. For instance, the *Linear Programming* (LP) relaxation plays a central role in approximate solvers. It is well known that solving the ILP is *NP-hard* problem. However, it could be relaxed to the polynomial-time solvable linear programming. Later, a fractional solution for the LP will be rounded to obtain a feasible solution for the ILP. Different rounding strategies define separate approximate solver techniques [119]:

- **Deterministic rounding** follows a predefined strategy.
- **Randomized rounding** performs a round-up of each fractional solution value to the integer uniformly.

In contrast to rounding, another technique requires building a *Dual Linear Program* (DLP) for a given linear program. This approach utilizes the *weak* and *strong duality* properties of DLP to derive the distance of the LP solution to the original ILP optimal solution. Other properties of DLP form a basis for the *Primal-dual* algorithms. They start with a dual feasible solution and use the dual information to derive the primal linear program solution (possibly infeasible). If the primal solution is not feasible, the algorithm modifies the dual solution increasing the dual objective function values. In any case, these approaches are far beyond the thesis scope, but in case of an interest reader could start his own investigation from [119].

**Heuristics.** As opposed to the solvers mentioned above, heuristics do not provide any guarantee on the solution quality. They are applicable not only to the white-box TS but also to the black-box cases. These approaches are sufficient to quickly reach an immediate, short-term goal in such cases, when finding an optimal solution is impossible or impractical because of the huge search space size.

As in the reviewed above approaches, here exist many facets for classification. We start from the largest one, namely the *level of generality*:

- **Simple heuristics** are the specifically designed to tackle the concrete problem algorithms. They fully rely on the domain knowledge, obtained from the optimization problem. Simple heuristics do not provide any mechanisms to escape a local optimum therefore, could be easily trapped to it [90].
- **Meta-heuristics** are the high-level heuristics that being domain knowledge-dependent, also provide some level of generality to control the search. They could be applied to broader range of the OPs. They are often nature-inspired and comprise mechanisms to escape the local optima but may converge slower than the simple heuristics. For the more detailed explanation we refer to survey [12].
- **Hybrid-heuristics** arise as the combinations of two or more meta-heuristics. They could be imagined as the recipes merge from the cookbook, combining the best decisions to create something new and presumably better.
- **Hyper-heuristics** are the algorithms that operate in the search space of *low-level heuristics* (LLH). Instead of tackling the original problem, they choose (or construct) LLHs, which will tackle this problem for them [21].

In the upcoming Section 2.2, dedicated to heuristics, we provide more detailed information on each of the approaches mentioned above.

### The Most Suitable Solver Type

“Fast, Cheap or Good? Choose two.”

---

*The old engineering slogan.*

At this point, we have reached the crossroads and should make a decision, which way to follow.

Firstly, we have the exact solvers for the optimization problems. As mentioned above, they always guarantee to derive an optimal solution. Today, tomorrow, maybe in the next century, but eventually the exact solver will find it. The only thing we need is to construct the exact algorithm. This approach definitely offers the best final solution quality however, it sacrifices the solver construction simplicity and the speed in problem-solving.

Secondly, we have the approximate solvers. They do not guarantee to find the one and only optimal solution but suggest a provably good instead. From our perspective, the required effort for constructing the algorithm and proving its preciseness remains the same as for the exact solvers. However, this approach outperforms the previous one in the speed of problem-solving, sacrificing a reasonably small amount of the result quality. It sounds like a good deal.

Finally, the remaining heuristic approaches. They quickly produce a solution, in comparison to the previous two. In addition, they are much easier to apply for the specific problem — there is no need to build complex mathematical models or prove the theorems. However, the biggest flaw in these approaches is the absence of the solution quality guarantee.

As we mentioned in Section 2.1.1, this thesis is dedicated to facing the practical combinatorial problems, such as the TSP. They are NP-complete, that is why we are not allowed to apply the exact solvers. In both approximate and heuristic solvers we are sacrificing the solution quality, though in different quantities. Nevertheless, the heuristic algorithms repay in the development time and provide the first results faster. The modern world is highly dynamic, in the business survive those, who are faster and stronger. In the most cases, former plays the crucial role for success. The great products are built iteratively, enhancing existing results step-by-step and leaving the unlucky decisions behind. It motivates us stick to the heuristic approach within the scope of the thesis.

In the following Section 2.2 we shortly survey different heuristic types and examples. We analyze their properties, weaknesses and ways to deal with them. As the result, we select the best-suited class of heuristics for solving the TSP problem.

## 2.2 Heuristic Solvers for Optimization Problems

We base our descriptions of heuristics and their examples on the mentioned in Section 2.1.1 traveling salesman problem. The input data  $X$  to our heuristics will be the problem description in form of a distance matrix (or coordinates to build this matrix), while as an output  $Y$  from heuristics we expect to obtain the sequence of cities, depicting the route plan.

Most heuristic approaches utilize the following concepts:

- **Neighborhood**, which defines a set of solutions that could be derived performing a single step of the heuristic search.
- **Iteration**, which could be defined as an action (or a set of actions) performed over the solution in order to derive a new, hopefully better one.
- **Exploration** (diversification), which is the process of discovering previously unvisited and presumably high-quality parts of the search space.
- **Exploitation** (intensification), which is the usage of already accumulated knowledge (solutions) to derive a new solution but similar to existing one.

### 2.2.1 Simple Heuristics

As we mentioned above, simple heuristics are domain-dependent algorithms, designed to solve a particular problem. They could be defined as the rules of thumb, or strategies to utilize the information, exposed by the TS and obtained from the previously found solutions, to control the problem-solving process [90].

Scientists draw the inspiration for heuristics creation from all aspects of our being: starting from the observations of how humans tackle daily problems using intuition, and proceeding to the mechanisms discovered in nature. The two main types of simple heuristics were outlined in [22]: *constructive* and *perturbative*.

The first type aggregates the heuristics which construct the solutions from its parts step by step. A prominent example of constructive approach is a *greedy algorithm*, which can also be called the *best improvement local search*. When applied to TSP, it tackles the path construction simply accepting the next closest city from currently discovered one. Generally, the greedy algorithm follows the logic of making a sequence of locally optimal decisions therefore, it ends up in a local optimum after constructing the very first solution.



The second type, called a *local search*, implies heuristics which operate on the complete solutions, perturbing them. A simple example of the local search is a *hill climbing algorithm*, also known as a *first improvement local search* [118]. This heuristic accepts a better solution as soon as it finds it, during the neighborhood evaluation. This approach plays a central role in many high-order algorithms however, it could be very inefficient, since in some cases the neighborhood could be enormously huge.

Indeed, since the optimization result is fully dependent on the starting point. The use of simple local search heuristics might not lead to a globally optimal solution. Nevertheless, in this case the advantage will be the implementation simplicity [119].

### 2.2.2 Meta-Heuristics

Meta-Heuristic (MH) is an algorithm, created to solve a wider range of complex optimization problems with no need to deeply adapt it to each problem.

The research in MHs field arose even before 1940s, when the MHs were already actively applied. However, there were no all-embracing and complex studies of MHs at that time. The first formal studies appeared between 1940s and 1980s. Deep and profound research in this field reaches its most active stage in the late 1990s, when the numerous MHs popular nowadays were invented. The period from 2000 and up till now the authors in [107] call the framework growth time, when the meta-heuristics widely appear in form of frameworks, providing a reusable core and requiring only the domain-specific adaptation.

The prefix *meta-* indicates the algorithms to be of the *higher level* when compared to simple problem-dependent heuristics. The static part of the algorithms is stable and problem independent, it forms the core of an algorithm and usually exposes *hyper-parameters*, which could be used for the algorithm configuration. The changeable parts are domain-dependent and should be adapted for problem at hand. Many MHs contain stochastic components, which provide abilities to escape from local optimum. However, it also means that the output of meta-heuristic is non-deterministic and it could not guarantee the result preciseness [18].

The meta-heuristic optimizer success on a given OP depending on the *exploration vs exploitation balance*. If there is a strong bias towards diversification, the solving process could naturally skip a good solution while performing huge steps over the search space, but in case of intensification domination, the process will quickly settle in the local optima. The disadvantage of the simple heuristic approaches mentioned above is a high exploitation dominance, since they simply do not have the components contributing to exploration. In most of the cases, it is possible to decompose MH into simple components and clarify, to which of competing processes contributes each component. Often, the simple heuristics are used as the intensification component.

In general, the difference between existing meta-heuristics lays in a particular way how they are trying to achieve this balance, but the common characteristic is that the most of them are inspired by real-world processes — physics [117], biology [103], ethology [34, 102, 110], and even evolution [11, 39].

### Meta-Heuristics Classification

When the creation of novel methodologies has slowed down, the research community began to organize and classify the created algorithms.

As an example, [15] highlights the following classification facets:

- The **walk-through search space method** could be either trajectory-based or discontinuous. The first one corresponds to a closed walk through the neighborhood where such prominent examples as *iterated local search* [81] or *tabu search* [50] do exist. The second one allows large



jumps in the search space, where the examples are such MHs as *variable neighborhood search* [54] or *simulated annealing* [69].

- The **number of concurrent solutions** could be either single or multiple. Such approaches as tabu search, simulated annealing or iterated local search are examples of algorithms with a single concurrent solution. Evolutionary algorithms [39], ant colony optimization [34] or particle swarm optimization [67] are the instances of algorithms with multiple concurrent solutions (the population of solutions).
- From the **memory usage** perspective, we distinguish those approaches which do and do not utilize the memory. Tabu search explicitly uses memory in form of tabu lists to guide the search, but simulated annealing is memory-less.
- The **neighborhood structure** could be either static or dynamic. Most local search algorithms, such as simulated annealing and tabu search are based on a static neighborhood. Variable neighborhood search is an opposite case, where various structures of neighborhood are defined and interchanged while the algorithm solves the OP.

There are many more classification facets, which are not in the scope of this thesis. Figure 2.3 illustrates the summarized classification including some characteristics and well-known meta-heuristic instances we did not mention.

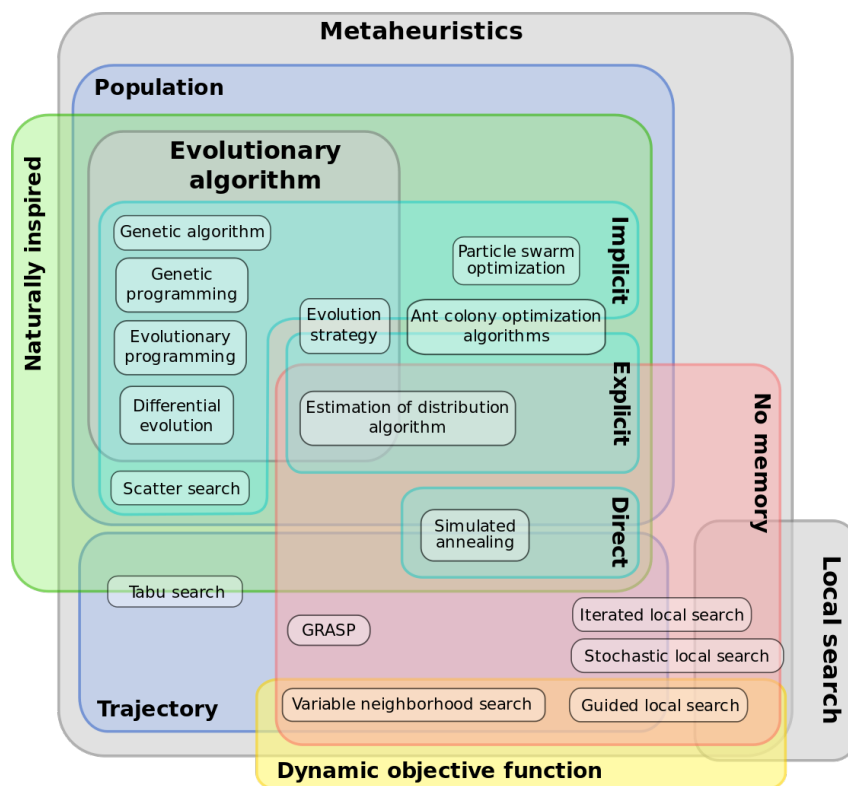


Figure 2.3 Meta-heuristics Classification [36].

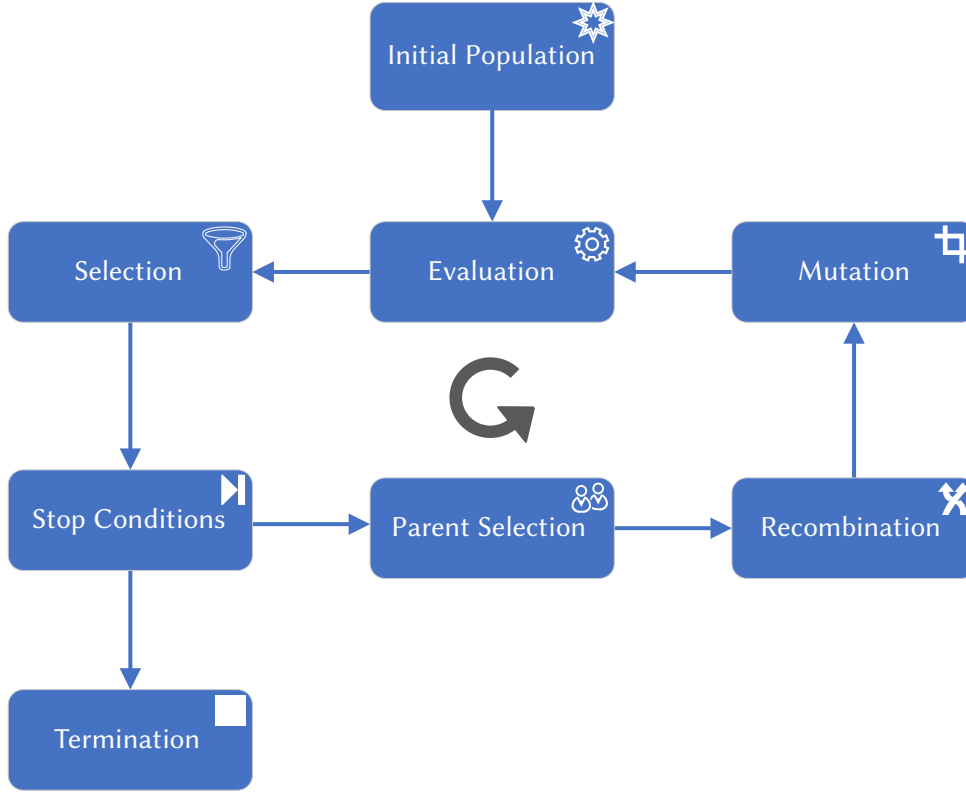


Figure 2.4 Evolutionary Algorithms Workflow.

### Meta-Heuristics Examples

At this point, let us briefly describe some of the most prominent and widely used meta-heuristics. It is motivated by the later usage of them in our approach, described in Section 4.4.

**Evolutionary Algorithms (EAs)** are directly inspired by the processes in nature, described in evolution theory. The common underlying idea in all of these methods is as follows: if we put a population of individuals (solutions) into an environment with limited resources (population size limit), a competition processes cause natural selection, where only the best individuals survive [39].

Three basic actions are defined as operators of EAs: a *recombination* operator selects the parent solutions, which later will be combined to produce the new ones (offspring); a *mutation* operator, when applied to solution, creates a new and very similar one. Applying both operators, the algorithm creates a set of new solutions — the offspring, whose quality is then evaluated with the TS. After that, a *selection* operator is applied to all available solutions (parents and offspring) to keep the population size within the defined boundaries. This process is repeated, until some termination criterion is fulfilled. For instance, the maximal iterations counter was reached, the number of TS evaluations exceeds the defined maximal value, or the solution with the required quality is found. The high-level work-flow of EA is depicted in Figure 2.4.

The well-known examples of EAs include the *genetic algorithm* [103], *genetic/evolutionary programming* [72], *evolution strategies* [11], and many other algorithms.

*Genetic Algorithm* (GA) is the first of all associated with the Evolutionary Algorithms. GA traditionally has a fixed workflow: given an initial population of  $\mu$  usually randomly sampled individuals, the parent selection operator creates pairs of parents, where the probability of each solution to become a parent

depends on its objective value (fitness, or results). After that, the crossover operator is applied to every created pair with a probability  $p_c$  and produces children. Then, newly created solutions undergo the mutation operator with an independent probability  $p_m$ . The resulting offspring perform a tournament within the selection operator and  $\mu$  survivals replace the current population [38]. Distinguishable characteristic of vanilla GA is the usage of the following operators: bit-string solution representation, one-point crossover recombination, bit-flip mutation and generational selection (only children survive).

*Evolution Strategy* (ES), comparing to GA, is working in a vector space of the solution representation. However, they also use the population size of  $\mu$  individuals and  $\lambda$  offspring generated in each iteration. While the general workflow for all EAs remains the same, they mostly differ in underlying operators. In ES, the parent selection operator takes a whole population into consideration uniformly, the recombination scheme could involve more than two parents to create one child. To construct a child, the recombination operator joins parents alleles in two possible ways: (1) with uniform probability for each parent (discrete recombination), or (2) averaging the weights of alleles by parent solution quality (intermediate recombination). There are two selection schemes, used in such algorithms.  $(\mu, \lambda)$ : discard all parents and select only among offspring highly enriching the exploration, and  $(\mu + \lambda)$ : include also the predecessor solutions into selection, which is often called the *elitist selection* [38]. In many cases, the ES utilizes a very useful feature of *self-adaptation*: changing the mutation step sizes at runtime, which we will discuss in Section 2.3.3.

**Simulated Annealing (SA).** This is the other type of meta-heuristics, inspired by the technique used in metallurgy to obtain ‘well-ordered’ solid-state of metal [117]. An annealing technique imposes a globally minimal internal energy state and avoids locally minimal semi-stable structures.

The SA treats the search process as a metal with a high temperature at the beginning and lowering it to the minimum while approaching the end. It starts with an initial solution  $S$  creation (randomly or using some other heuristic) and temperature parameter  $T$  initialization. At each iteration, a new solution candidate is sampled within a neighborhood of the current solution:  $S^* \leftarrow N(S)$ . The newly sampled solution replaces the older one, if (1) optimization objective  $f(S^*)$  dominates over  $f(S)$  or (2) with a probability that depends on a quality loss and current value of  $T$ , see Equation (2.1).

$$p(T, f(S^*), f(S)) = \exp\left(-\frac{|f(S^*) - f(S)|}{T}\right) \quad (2.1)$$

At each iteration the temperature parameter  $T$  value is decreased following some type of annealing schedule, which is also called *cooling rate* [18]. The weak side here is that the quality of each annealing schedule is the problem-dependent and cannot be determined beforehand. Nevertheless, the SA algorithms with adaptive parameters do exist and address this problem changing the cooling rate or temperature parameter  $T$  during the search process. Later, we will shortly review these techniques in Section 2.3.3.

### 2.2.3 Hybrid-Heuristics

The hybridization of different systems often provides a positive effect — taking the advantages of one system and merging them with characteristics of the other, getting the best from both systems. The same idea is applicable in the case of meta-heuristics. Imagine you have two algorithms, one is biased towards exploration, the other — towards exploitation. Applying them separately, the expecting results in most cases may be far away from the optimal as the outcome of disrupted diversification-intensification balance. However, when merging them into, for example, repeated stages of hybrid heuristic, one will obtain the advantages of both escaping a local optimum and finding a good quality result.

Most of the available hybridization algorithms are created with the help of this idea of two heuristics staging combination, one of which is suited for the exploration and other is better for the exploitation.

The methods to construct the hybrids are mostly defined by the underlying heuristics. Therefore, to the best of our knowledge they could not be generalized and classified in an appropriate way. Commonly, there is only one shared characteristic in the usage of a *staging approach*, in which the output of one algorithm is used as the initial state of the other.

As during the simple heuristics review, here we also introduce examples of performed hybridization in order to provide the reader a better understanding how can be combined different algorithms components and what is the effect on the aforementioned balance.

### Hybrid-Heuristics Examples

**Guided Local Search and Fast Local Search.** The main focus of guided local search (GLS) in this case, lies in the search space exploration and the process guidance using incubated information. To some extent, the GLS approach is closely related to the frequency-based memory usage in tabu search. During the runtime, GLS modifies the problem cost function to include penalties and passes this modified cost function to the local search procedure. These penalties form a memory that characterizes a local optimum and guide the process out of it. The more time algorithm spends in the local optimum, the higher are the penalties. A local search procedure is carried out by fast local search (FLS) algorithm, where the main advantage is a quick neighborhood traversal. It is done by breaking it up into a number of small sub-neighborhoods. Afterwards, while performing the depth-first search over these sub-neighborhoods, it ignores those, which do not make any improvements. At some point in time, FLS reaches the local optimum and passes back the control in GLS to update the penalties and repeat the iteration [114].

**Direct Global and Local Search.** This hybridization consists of two stages: the stochastic global coarse pre-optimization and the deterministic local fine-optimization. At the first stage, the authors apply one of the two abovementioned meta-heuristics — genetic algorithm or simulated annealing [56]. A transition from global to local search happens after reaching the predefined conditions. For instance, when the number of TS evaluations exceeds a boundary, or when no distinguishable improvement was made in the last few iterations. Then, the pattern search algorithm also known as the direct, derivative-free, or black-box search performs fine-optimization. The hybrid-heuristic terminates when the pattern search converges to the local optima [109].

**Simulated Annealing and Local Search.** After the brief explanation of the previous two hybrids, it is not so difficult to guess, how the next hybridization works. The authors in their work [83] called this method ‘Chained Local Optimization’. Therefore, it is yet another representative of staged hybridization. Iteration starts with the current solution perturbation, called *kick* in [83], referring to a dramatic change of a current position within the search space. Afterwards, the hill climbing algorithm is applied to intensify the obtained solution. After reaching the local optimum, hill climber passes the control flow back to the simulated annealing for acceptance criteria evaluation, which finishes the iteration.

**EMILI.** Easily Modifiable Iterated Local search Implementation (EMILI) is a framework system for the automatic generation of new hybrid stochastic local search algorithms [89]. EMILI is a solver for permutation flow-shop problems (PFSP), also known as flow shop scheduling problems [96]. In PFSP the search of an optimal sequence of steps to create products within a workshop is performed. In this framework, the authors have implemented both generic algorithmic- and problem-specific building blocks. They also have defined grammar-based rules for those blocks composition and used an automatic

parameter tuning tool called IRACE [79] in order to find the high performing algorithm configurations. The workflow of EMILI could be split into three steps: (1) adaptation of the grammar rules to specific PFSP objective representations (makespan, sum completion times and total tardiness), (2) generation of all possible hybrid heuristics for each PFSP representation and (3) execution of IRACE to select the best-performing hybrid for each problem.

From our perspective, the described approach of automatic algorithm generation is an example of construction hyper-heuristics, which we describe in the upcoming Section 2.2.5. However, we are not authorized to change the system class (from hybrid- to hyper-heuristic) defined by the EMILI authors.

### 2.2.4 No Free Lunch Theorem

At this point, an obvious question may arise: “If there already exist excellent and well-performing heuristics, is there any need to put an effort into developing new algorithms instead of using existing ones?” The answer to this question is quite simple — the perfect algorithm suited for *all* OP does not exist and cannot exist at all. The empirical research has shown that some meta-heuristics perform better with some types of problems, but are less-performing with others. In addition to that, for different instances of the same problem type, the same algorithm could result in unexpected performance metrics. Moreover, even at different stages of the same problem solving process the dominance of one heuristic over another could change.

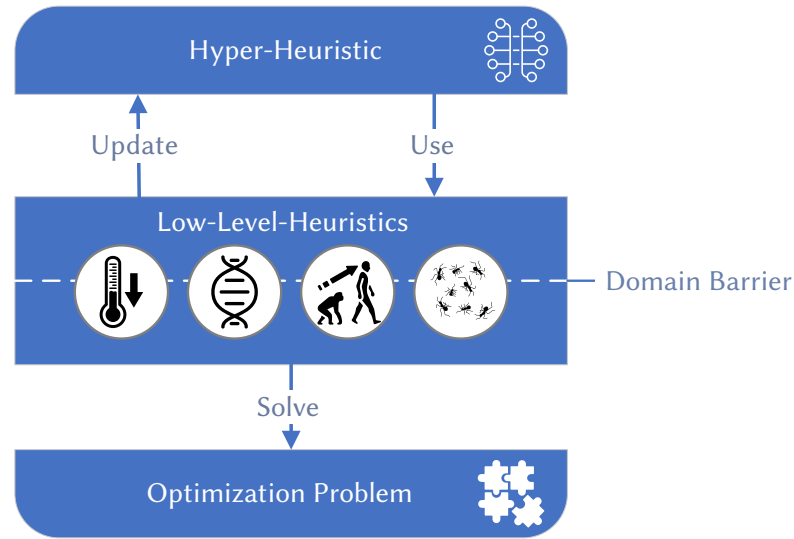
All search algorithms perform exactly the same, when the results are averaged over all possible optimization problems. If an algorithm is gaining the performance in one problem class, it loses in another class. This is a consequence of a so-called *no free lunch theorem for optimization* (NFLT) [121].

In fact, one cannot predict, how exactly one or another algorithm will behave with a problem at hand. A possible and most obvious way is to probe one algorithm and compare its performance to another one during the problem-solving process. In this case, simple heuristics and meta-heuristics are out of the competition, since once the optimization problem is solved, one probably would not try to solve it for the second time. Here, the *hyper-heuristics* come into play to intelligently pick heuristics suitable to the problem at hand. We will proceed with their description outlining the way they deal with the NFLT consequences in the following section.

### 2.2.5 Hyper-Heuristics

Many of state-of-the-art heuristics and meta-heuristics are developed in a complex and very domain-dependent way, which causes problems with their reuse. It motivated the research community to raise the question of a generality level at which the optimization systems can operate and still provide good quality solutions for various optimization problems.

The term **hyper-heuristic** (HH) was defined to describe an approach of using some *high-level-heuristics* (HLH) to select over other *low-level-heuristics* (LLH) and apply them to solve the *class* of optimization problems rather than a particular instance. Indeed, scientists report that the combination of different HLH produces better results when applied separately [35]. This behavior can be explained by the way of how the search process evolves in time. When one applies a heuristic, it sooner or later converges to some extreme point, hopefully global optimum. But it is ‘blind’ to others, not visited regions of the search space. Changing the trajectory of an investigation by (1) drastically varying the neighborhood, (2) changing the strategy of neighborhood exploration and exploitation could (1) bring one to those previously unreachable zones (2) in more rapid ways. However, usually it is hard to predict how one LLH will behave in every stage of the search process in comparison to another. In hyper-heuristics, this job was encapsulated into the HLH and performed automatically.



**Figure 2.5** Hyper-Heuristics.<sup>a</sup>

<sup>a</sup>Icons are taken from <https://thenounproject.com/>

In [86] the authors made an infer that HHs can be viewed as a form of reinforcement learning (RL), which is a logical conclusion, especially if rephrased to *hyper-heuristics utilize reinforcement learning methodologies*.

The new concept, which was implicitly used in meta-heuristics, but explicitly pointed out in hyper-heuristics is the *domain barrier* (see Figure 2.5). As was stated previously, HH do not tackle the OP directly, but use LLH instead. This means that usually HH is minimally aware of the domain details, such as data types, relationships, etc. within a domain. This information is rather encapsulated in LLHs, therefore, HHs could be applied to a broader range of optimization problems.

With this idea, many researchers started to create not only hyper-heuristics to tackle a concrete optimization problem class, but also frameworks with building blocks for their creation.

## Classification

Although the research in hyper-heuristics field is actively going on, many algorithm instances were already created and some trials to organize approaches were conducted in [22, 35, 68, 101].

Researchers in their surveys classify HHs by different characteristics, some of which overlap, but sometimes important features (from our perspective) were not highlighted in all works.

In this section we unite of those important hyper-heuristics classification facets in order to better justify the goal of this thesis.

To begin with, there are two broadest classes, which differentiate HH *routine*, also called *nature of high-level-heuristic search space* [22, 23, 35]. The first class consists of hyper-heuristics to *select* low-level-heuristic, in other words *selection hyper-heuristic*. Please note, previously in this thesis all discussions of HHs were referencing to this specific type. These algorithms operate in the defined by complete and rather simple low-level-heuristics search space. The task of HLH here is to pick the best-suited LLH (or sequence of LLHs) based on the available prior knowledge and apply it to the OP underway. Hyper-heuristic of the second class seeks to *construct* LLH following some predefined receipt and using the atomic components of other heuristics as Lego bricks. The other commonly used name here is a *construction hyper-heuristic*. These approaches often lead to a creation of new and unforeseen heuristics



that are expected to reveal good performance while solving the problem at hand.

Next, the distinction in the *nature of LLH search space* arises. In other words: “How does the LLH derive a solution for the OP?” The authors in [22, 23, 35] distinguished *construction* LLHs, where the solution creation happens each time from scratch and *perturbation* LLHs, where the new solutions are created from parts of already existing ones.

The other broadly used characteristic is *learning time*. From this perspective hyper-heuristic can be of type *online*, *offline* or *not learning* algorithm [22, 101]:

- In **online** case, the HH derives information, used to select among LLH, while those LLH are solving the problem.
- In **offline** case, the learning happens before solving a certain OP. Here one should first train the HH solving other homogeneous problem instances by underlying LLHs (offline learning phase). After that, the HH will be able to properly choose among LLHs, therefore, be applicable to problems at hand (online use phase). Note that this approach also requires creation of a meta-features extraction mechanism and its application to every optimization problem.
- In the last case **no learning** mechanisms are present. Therefore, HH here performs to some extent a random search over LLH search space. At the first sight it may seem to be a weak approach, however, there exist meta-heuristics, which are similar to HH and perform well (variable neighborhood search).
- There also exist **mixed** cases, where the learning happens firstly in the offline and later also in the online phase. Definitely, it is a promising (in terms of results quality) research direction, despite its high complexity.

For more detailed analysis, description, other classification facets and respective hyper-heuristic examples we encourage the reader to look into recent classification and surveying researches [21, 22, 35, 101].

### Hyper-Heuristics Instance Examples

**Hyper-heuristic for integration and test order problem (HITO).** HITO [52] is an example of a construction HH. LLHs in this case are presented as a composition of basic EAs operators — crossover and mutation forming multi-objective evolutionary algorithms (MOEA). HH selects those components from *jMetal* framework [37] using interchangeably *choice function* (form of the weighted linear equation) and multi-armed-bandit-based heuristic to balance exploitation of good components and an exploration of new promising ones.

**Markov Chain Hyper-Heuristic (MCHH).** MCHH [84] is an online selection hyper-heuristic for multi-objective continuous problems. It utilizes reinforcement learning techniques and Markov chain approximations to provide an adaptive heuristic selection method. While solving the OP, MCHH updates the prior knowledge about the probability of producing Pareto dominating solutions by each underlying LLH using Markov chains, guiding an LLH selection process. Applying online reinforcement learning techniques, this HH adapts transition of weights in the Markov chains constructed from all available LLHs, updating prior knowledge for LLH selection.

## Hyper-Heuristics Frameworks Examples

**Hyper-Heuristics Flexible Framework (HyFlex).** HyFlex [87] is a software skeleton, built specifically to help other researchers creating hyper-heuristics. It provides the implementation of components for 6 problem domains: boolean satisfiability, bin packing, personnel scheduling, permutation flow shop and vehicle routing problems. Thereby, problem and solution descriptions, evaluation functions and adaptations for set of low-level-heuristics are provided out-of-the-box. The set benchmarks and comparison techniques to other built HHs on top of HyFlex are included in the framework as well.

The intent of HyFlex creators was to provide low-level features that enable the users to focus directly on HLHs implementation without a need to challenge other minor details. It also brings a clear comparison among created HLH performance, since the other parts are mostly common.

From the classification perspective, all derivatives from the HyFlex framework are selection hyper-heuristics, however, they utilize different learning approaches. Algorithms, built on top of HyFlex framework could be found in many reviews [35, 85, 101] or on the CHeSC 2011 challenge website<sup>1</sup> (CHeSC is dedicated to choosing the best HH built on top of HyFlex).

Along with HyFlex, the number of hyper-heuristic-dedicated frameworks is growing, some of them are under active development while others are abandoned:

- **Hyperion** [108] is a construction hyper-heuristic framework, aiming to extract information from the OP search domain for identification of promising components in form of object-oriented analysis.
- **hMod** [116] framework allows not only to rapidly prototype an algorithm using provided components, but also to construct those components using predefined abstractions (such as *Iterative-Heuristic*). In the current development stage, developers of hMod are focusing on a creation of development mechanisms rather than providing a set of pre-built heuristics.
- **EvoHyp** [92] framework focuses on hyper-heuristics, created from evolutionary algorithms and their components. Here, the authors enable framework users to construct both selection and generation HHs for both construction and perturbation LLHs types.

### 2.2.6 Conclusion on Heuristic Solvers

To conclude our review on heuristic approaches for solving optimization problems, we shortly refresh each heuristic level.

On the basic level remain simple heuristics with all their domain-specific knowledge usage and particular tricks for solving problems. Usually, they are created to tackle a concrete problem instance, applying simple algorithmic approach. The simplicity of development and usually fast runtime result in medium-quality results.

On the next level inhabit meta-heuristics. They could be compared with more sophisticated solutions hunters, which could not only charge directly, but also take a step back when stuck in a dead end. This additional skill enables them to survive in new and complex environments (optimization problems). However, some adaptations to understand a specific problem and parameter tuning for better performance still should be performed.

Along with MHs exist hybrid-heuristics. In short, they simply just took some survival abilities from several meta-heuristics with a hope to outperform and still requiring adaptation and tuning. In some cases this hybridization provides an advantage, but as the time shows they did not force MHs out.

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<sup>1</sup>Cross Domain Heuristic Search Challenge website: [asap.cs.nott.ac.uk/external/chesc2011/](http://asap.cs.nott.ac.uk/external/chesc2011/)

Therefore, we can conclude that the provided balance between development effort and exposed results' quality not always assure users to use them.

Finally, those who lead the others, hyper-heuristics are on the upper generality level. Operating by the other heuristics, HHs analyze how good the former are and make a use of this knowledge by solving a specific problem using those best-suited heuristics. Imposing such great abilities, hyper-heuristics tackle not only a certain optimization problem but an entire class of problems.

## 2.3 Setting Algorithm Parameters

Most of the existing learning algorithms expose some parameter set, needed to be assigned before using this algorithm. Modifying these parameters, one could change the system behavior and a possible result quality.

When we are talking about the problem of settings the best parameters, the following terms should be outlined explicitly:

1. **Target System (TS)** is a subject whose parameters are undergoing changes. In short, it could be a heuristic, machine learning algorithm or any other system.
2. **Parameter** is one of the configuration hooks, exposed by TS. It should be described in terms of its type and possible values.
3. **Configuration** is a unique combination of parameter values, required to run TS.
4. **Search Space** is a set of all possible Configurations for defined parameters.

In this thesis we use notions of *parameter* and *hyper-parameter* interchangeably, since the approaches discussed in this section are generally applicable also in machine learning cases. As an example, consider a neuron network. Hyper-parameters in this case specify a structure (number of hidden layers, units, etc.) and define a learning process (rate, regularization parameters values, etc.). Changes in their values dramatically affect the networks' performance and results.

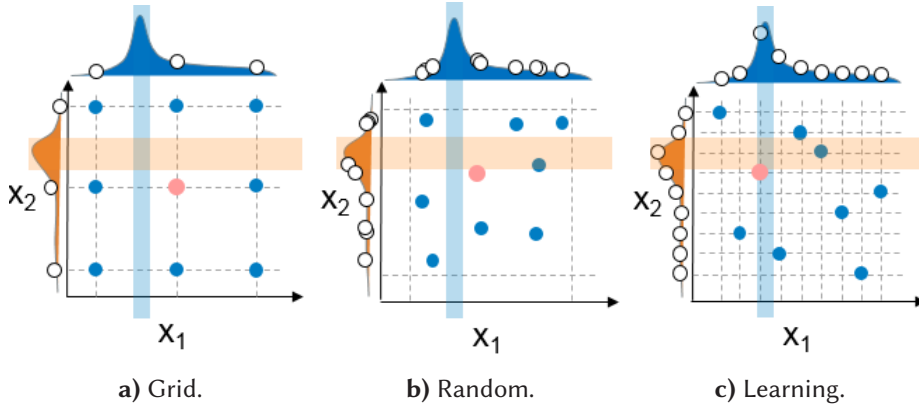
A frequently tackled optimization problem is a *parameter settings problem* (PSP): the process of searching hyper-parameter values that optimize some characteristic of TS. When talking about NN example, PSP could be defined as a task of networks' accuracy maximization with a given dataset, resulting in a single-objective PSP (SO-PSP). Optimizing a number of TS characteristics simultaneously, such as training time and prediction accuracy, one transforms the SO-PSP into a multi-objective PSP (MO-PSP).

The same applies to heuristics. A proper assignment of hyper-parameters has a great impact on the exploration-exploitation balance and, as a result, on an overall algorithm performance [74].

Up until now, there were formalized many approaches for solving task of settings hyper-parameters. One way is simply to use the intuition and to apply the parameters that seem more or less logical for a particular system and a problem instance. This error-prone technique was quickly abandoned in favor of automatic approaches. It was also motivated by increasing computational capacities, which gave an opportunity to evaluate more configurations in less time. These automatic methods could be split into two technique families: one is an offline *parameter tuning*, which is performed at the design time and the other is an online *parameter control*, performed at runtime.

### 2.3.1 Parameter Tuning

Roughly speaking, the offline approach is a process of traversing the search space of hyper-parameters and evaluating TS with these parameters on some set of toy problems. At the end of this process, the



**Figure 2.6** Automated Parameter Tuning Approaches.

best found HPs are reported and later used to solve a new, unforeseen problem instance.

In this part of thesis we outline existing automated approaches for parameter tuning, illustrating them in Figure 2.6<sup>1</sup>. In this example, the TS exposes two parameters:  $X_1$  and  $X_2$ . Each figure shows dependencies between  $X_1$  (horizontal axis) and  $X_2$  (vertical axis) values and the subject of optimization along those axes (here the maximization case is depicted). The best configurations found by each approach are highlighted in pink.

**Grid search parameter tuning.** It is a rather simple approach for searching parameters. Here, the original search problem is relaxed and later solved by a brute-force algorithm. The set of all possible configurations (parameter sets) for relaxed problem is derived by specifying a finite number of possible values for each hyper-parameter under consideration. After evaluating all configurations on TS, the best-found solution is reported. Hence, this approach could skip promising parts of search space (Figure 2.6a). Moreover, the required time to probe all possible combinations is increasing by means of a factorial complexity.

**Random search parameter tuning.** This methodology relies on a random (often uniform) sampling of hyper-parameters and their evaluation on each iteration. At first sight, it might seem unreliable to chaotically traverse the search space. But empirical studies show that with a growing number of evaluations this technique starts to outperform grid search [9]. As an example, let us draw your attention to the best configurations (highlighted in pink) found by grid (Figure 2.6a) and random search (Figure 2.6b) techniques. The best randomly sampled configuration is definitely better than the one found by the grid search.

**Heuristic search parameter tuning.** By their nature, heuristic algorithms may be applied to tackle the most black-box search problems. Since the parameter tuning is one concrete type of search problem, it is also often tackled by a high-order heuristic approaches (meta-, hybrid-, hyper-heuristics) [25, 29, 30]. The advantage of heuristics usage lays in their ability to learn during the optimization process and use an obtained memory to guide the search more efficiently.

**Model-Based Search Parameter Tuning.** In most cases, the dependencies between tuned parameter values and optimization objective do exist and can be utilized for hyper-parameter tuning. By predicting

<sup>1</sup>Original graphics are taken from [70]

which parameter combinations lead to better results, model-based tuning could make precise guesses. As it is shown in Figure 2.6c, after accumulating enough information the learning algorithm starts making more precise guesses, which in contrast to previously outlined model-free approaches are desirable and more robust.

Naturally, this optimization problem could be tackled by almost every approach discussed in this thesis. However, taking into account the fact that (1) TS is often a *black-box* we eliminate exact and approximate solvers, (2) the evaluation cost is high, therefore, it is not desirable to apply the aforementioned heuristics directly, since they require performing a high number of TS evaluations to find a good configuration. With this idea in mind, researchers started to (1) create optimization algorithms that traverse the search space of configurations more efficiently and (2) build models that could imitate the dependencies between parameters and objective values, a so-called *surrogate models*. The former direction is nothing else but an enhancement to already existing optimization techniques, which allows accumulating and utilization of more information, obtained during an optimization. The latter approach is crucial for problems where TS is expensive to evaluate. It is often used as an enhancement in optimization algorithm, enabling one to simulate evaluation of real system instead of expensive direct evaluations. Still, it is a frequently used approach to combine the previously reviewed search space traversal techniques, such as evolutionary algorithms, simulated annealing, tabu search with the surrogate models for optimization.

### 2.3.2 Systems for Model-Based Parameter Tuning

Parameter tuning is an obligatory task when the maximum system performance is a must-have requirement and should be performed at the design time. Novel tuning approaches are usually developed in form of frameworks with exposed hooks for attaching the TS.

Since the target system evaluations here supposed to be costly, parameter tuning frameworks are trying to utilize every single bit of information from evaluations and a creation of surrogate models and using efficient optimization approaches is obligatory.

In this section we review some existing open-source parameter tuning systems from the following perspectives:

- **Conditional parameters support** is provided to user and handled by tuning system ability to describe conditional dependencies between hyper-parameters. As an example, imagine *crossover type* parameter of genetic algorithm that takes only some specific values: partially mapped crossover (PMX), Cycle Crossover (CX), etc. Binding a certain crossover type, one will require providing parameters for this specific crossover type, as well as to eliminate the respective parameters for other crossover types. This type of dependency could be described in form of a parent-child relationship, however, other types of dependencies also exist.
- **Parameter types support** is one of the basic tuning systems usability requirements. In detail, TS parameters could be not only a numerical (integer or fractional) but also a categorical in form of strings, boolean values, etc. Considering categorical data types, they could be either *nominal*, which depict only possible atomic values, or *ordinal*, which imply also value comparison but no distance notion. For instance, let us refer to genetic algorithm parameters. *Population size* is of numerical integer type in a range  $[1..∞)$ , *mutation probability* is of numerical fractional type in a range  $[0..1]$ , *crossover type* is of categorical nominal type with {PMX, CX} choices. Please note, we could also view the population size as a set of finite values {10, 100, 1000} therefore, turning it into the categorical ordinal parameter.



- **Extensibility** is crucial when one would like to try a new promising and intriguing learning algorithm for guiding a search that was not available in the parameter tuning system yet. Practically, one may need not only new learning algorithm, but some other features like a non-trivial stopping criterion, tools for handling stochastic behaviors, or different strategies for random sampling (which are used to replace a model-based prediction, while the tuning system is learning).
- **Parallel evaluations** required for utilizing available computational resources that could scale horizontally, providing simultaneous evaluation of multiple configurations. This often could speeds-up the learning process.

Among reviewed systems, we could distinguish those, which were created directly to face the parameter tuning problem and the others that are more generic optimizers but still applicable in parameter tuning cases. A specific optimizer will be used for searching the parameters, if it exposes several features. Firstly, it must consider an optimization function evaluation to be expensive and tackle this problem explicitly. For instance, using surrogate models or the other TS approximations. Secondly, a potential tuner should be able to tackle dependencies and conditions among parameters.

### SMAC

Sequential Model-based Algorithm Configuration (SMAC<sup>1</sup>) [58] is a system for parameters tuning, developed by the AutoML research group (here we review the 3<sup>rd</sup> version of SMAC).

In their research, scientists generalized the process of parameter tuning under the *Sequential Model-Based Optimization* (SMBO) term as the iterations between (1) fitting models and (2) using them to choose the next configurations for evaluation. This term naturally formalizes most of the existing (except MBMO, but we do not tackle multi-objectiveness in this thesis) parameter tuning approaches and may be used as a distinguishing characteristic of optimization algorithms, since they naturally could be applied not only to the parameter tuning problems.

SMACv3 is an extension introducing the learning models and sampling mechanisms to previously existing random online aggressive racing (ROAR) algorithm. The authors showed that a machine learning in general and regression models in particular (playing the role of surrogates) are applicable not only to parameter tuning but also to optimize any expensive black-box function.

The development of this system was motivated by the limitations of all existing SMBO approaches. Among them an expanding the applicability to categorical, but not only to numerical parameters. Also, to reduce a variance influence the target algorithm performance optimization may be performed on a number of problem instances (benchmark set), instead of a single instance.

A routine in SMAC could be viewed as an iterated application of three steps: (1) building a learning model, (2) using it for making choices regarding which configurations to investigate next and (3) actual evaluation of TS.

The evaluation (3) here is carried out by the original ROAR mechanism, where the running of each new candidate solution continues until enough data (from benchmark set of problem instances) is obtained to either replace the current solution or reject the candidate. On contrary to model-less ROAR, SMAC at step (1) builds the regression random forest surrogate — an instance of a machine learning algorithm [19]. The usage of the regression decision trees is motivated by the fact that they fit well to categorical data and complex dependencies in general. Later, at step (2) an iterative local search (ILS) heuristic is applied in combination with *expected improvement* (EI) evaluation (part of the Bayesian optimization process) [105]. The EI is a measurement of possible solution quality improvement obtained by an underlying configuration, therefore, higher EI means that the candidate is better. ILS

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<sup>1</sup>SMACv3 GitHub repository <https://github.com/automl/SMAC3/>



starts at the best previously found configuration and traverses its neighborhood distinguishing between configurations using EI and regression model built at step (1). SMAC compares configurations by means of the objective value and considers only minimization case. EI is large for those configurations, which have a low predicted cost and for those, with high uncertainty in results, therefore, providing the exploration-exploitation balance [62].

## IRACE

IRACE<sup>1</sup> is a hyper-parameter tuning package [79] as the implementation of the iterated racing algorithm [16].

The underlying methodology is somewhat similar to the one implemented in SMACv3 and comprise three main steps: (1) sampling new configurations using prior knowledge, (2) empirically finding the best ones among the sampled using the racing algorithm and (3) updating the prior knowledge to bias future samples towards better configurations. The prior knowledge here is represented as a probability distribution of values for each parameter independently (truncated normal and discrete distributions for numeric and categorical parameter types respectively). During step (3), the probability distributions are build using the best found in step (2) configurations, increasing the sampling chance for promising values.

Iterated racing step (2) here is a process of running the target system using sampled configuration on a set of problem instances. After solving each instance, the statistically worse-performing configurations are rejected and racing proceeds with remaining ones. This process continues until it reaches the predefined number of survivors, or after solving a required amount of problem instances (in this case all remaining configurations are considered to be good).

IRACE supports various data types, such as numerical or categorical and the possibility of conditions description as well. While the problem of data types is resolved by the usage of different underlying distribution types, the conditional relationships are handled by the dependency graphs. During step (1), non-conditional parameters are sampled firstly and only afterwards, if the respective conditions are satisfied, the dependent parameters are sampled.

## HpBandSter

A distributed Hyperband implementation on Steroids (HpBandSter<sup>2</sup>) is a realization of BOHB algorithm [41] in the software framework. While SMAC outperforms and partially reuses the decisions made in ParamILS [59], BOHB (Bayesian optimization combined with Hyperband) is the parameter tuning tool that outperforms SMAC and was created by the same AutoML research group.

As it stated in the framework name, the SMBO routines are carried out with mainly two algorithms: learning and configurations sampling is performed by the Bayesian optimization (BO) technique *tree parzen estimator* (TPE), while evaluation of sampled configurations and their comparison is carried out by the Hyperband (HB) algorithm.

The TPE usage instead of naive Gaussian processes-based BO and expected improvement evaluation was motivated by a better dimensional scaling abilities and an internal support of both numerical and categorical parameter types. However, some minor transformations are still required. Unlike vanilla BO, where the optimization is done by modeling the result distributions given the configuration parameters, TPE builds two distributions of parameter values. It splits the configurations into two sets distinguishing their ‘goodness’. During the sampling, it proposes those parameter values, which have a high probability

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<sup>1</sup>IRACE GitHub repository <https://github.com/MLopez-Ibanez/irace>

<sup>2</sup>HpBandSter GitHub repository: <https://github.com/automl/HpBandSter>

to be in the ‘good’ distribution and simultaneously low probability to be in the ‘bad’ one. For more detailed explanation, we refer to TPE description given in [10].

A central part of BOHB, namely the Hyperband algorithm, is a promising bandit-based strategy for hyper-parameter optimization [77], in which the *budget* for entire parameter tuning session is defined beforehand and divided between iterations. The role of the budget could play any setting that controls the accuracy of a configuration evaluation by TS, where estimation with the maximal budget provides the most precise evaluation, while the minimal budget gives the least accurate approximation of configuration results. The running examples of budget could be a number of iterations in iterative algorithm, a number of epochs to train the neuron network, or a number of problem instances from benchmark set to evaluate. As a result, the requirements in TS arise to expose and support budget usage as expected in BOHB.

At each iteration, in original version HB samples a number of configurations uniformly at random. The authors introduced an *intensification* mechanism according to which, a number of per-iteration sampled configurations decreases for the later iterations, while the amount of budget given for iteration remains the same. As an outcome, first iterations of HB are full of coarse-grain evaluated configurations, while the later iterations produce a higher number of more precise measurements. Each iteration of HB is split to the number of *successful halving* (SH) procedure executions, which at each execution drop poorly performing configurations (usually  $2/3$ ). As one may expect, since the number of measured configurations in subsequent iterations decreases, the amount of SHs execution drops too, therefore, the remaining configurations are evaluated more precisely.

The binding of Hyperband and Bayesian TPE is made in several places. Firstly, the learning models are updated each time, when new results are available for every budget value. Secondly, at each HB iteration instead of random sampling, the TPE model is used to pick next configurations. Please note that BOHB uses only the surrogate, which was built on the configurations evaluated with the largest budget. This decision results in more precise surrogate models and, therefore, better predictions in the later stages of parameter tuning process.

### BRISEv2

The great part of software potential lays not only in its ability to tackle a problem at hand, but also on the general usability and adaptivity to unforeseen tasks. Here we review the 2<sup>nd</sup> version of BRISE<sup>1</sup> [93], since the very early BRISE versions (major version 1 [94]) were more monolithic and hard to apply for parameter tuning problem at hand.

While designing this system, authors were focused not solely on learning mechanisms for parameter prediction, but on the overall system modularity as well. Being a software product line (SPL), BRISE was designed as a set of interacting components (nodes), each acting according to its own specific role. The system could be viewed from two perspectives. One is a birds-eye view on all available nodes with their roles and the other is a fine-grained description of *main-node* concretely.

Before reviewing each perspective, it is worth justifying the central terms used in the system. Please note that some of them are similar to the one defined above, but they were explicitly implemented in form of interacting entities.

- **Experiment** encapsulates the information about a certain run of BRISE. For instance, within a parameter tuning session it carries such information as BRISE experiment description (a specification of parameter tuning procedure in JSON format), evaluated during session configurations with their results.

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<sup>1</sup>BRISEv2 GitHub repository: <https://github.com/dpukhkaiev/BRISE2/releases/tag/v2.3.0>

- **Configuration** is a combination of input parameter values for TS. It could be run several times to obtain a statistical data, therefore, contains number of *Tasks*. Naturally, the configurations are comparable in terms of the results averaged over performed runs.
- **Task** is a single evaluation of TS under provided configuration for specified in description problem scenario.
- **Parameter** is a meta-description of certain configuration part and a building block for search space. It defines a set or range of possible values.
- **Search space** comprises all parameters and their dependencies and could verify the validity of configuration.

From a birds-eye view perspective, BRISE consists of *main-node* as the system backbone, several *worker-nodes* as target algorithm runners under provided configurations, *event-service* to distribute tasks between available worker-nodes, *front-end-node* to control and report optimization process on a web-page, and non-obligatory *benchmark-node* that could be handy for executing and analyzing a number of experiments.

The main-node is a combination of objects, which interact in terms of queue callbacks. Therefore, when a new configuration is evaluated, the new model is built and used for the next configuration prediction. The intent of introducing the aforementioned terms is to use them as a core of the framework, while such components as *prediction models*, *termination criteria*, *repetition management* or *outliers detection* are exposed to client for the variability reasons. Naturally, the developers also created a set of available out-of-the-box implementations for each variability component.

To use BRISE for parameter tuning, one should (1) construct an experiment and search space descriptions in JSON format and (2) add the respective target system evaluation logic in *workers*. All the rest will be carried out by the system.

### 2.3.3 Parameter Control

Generally speaking, the biggest disadvantage of parameter tuning approaches is defined by the fact that they usually require many TS runs to evaluate its performance with different configurations. On the other hand, the parameter control approaches are able to solve this issue but the drawback lays in their universality.

The advantageous characteristic of any system is its ability to adapt at runtime. It could happen so that an algorithm with tuned parameters performs well at the very beginning of a problem-solving process, but struggles in the later stages. The other algorithm configuration may result in an opposite behavior. This could be caused by various reasons and it is often hard to tell, which of them the algorithm is facing at the moment.

In contrast to the parameter tuning approaches, where optimal parameters are *firstly* searched and only afterwards are used to solve the OP, the parameter control is an approach of searching the parameters *while* solving the OP. It also could be expressed as a system reaction to the changes in a solving process. Sometimes, it is named an *online* parameter tuning. The drawback of this approach lays in a lack of generality, since often a parameter control technique is embedded into an algorithm, therefore, is algorithm-dependent.

The only broad classification facet we were able to distinguish is the *type of control mechanism*, where the *deterministic* and *adaptive* strategies exist. The first type suggests changing the parameters in a predefined schedule, while the second type assigns the parameter values upon received feedback. To the best of our knowledge, the adaptive approaches are mostly dependent on the concrete algorithm

instance. Therefore, it is hard to present a generic classification of parameter control approaches for all algorithms. However, this could be done for each particular algorithm family.

We provide an insight into the parameter control reviewing the examples of proposed strategies for some meta-heuristics. For the more comprehensive review of the recently published strategies we encourage the reader to examine the source paper, used here [57].

### Parameter Control in Simulated Annealing

The most frequently controlled parameters in simulated annealing algorithms are the *cooling rate* (the velocity of temperature decrease) and the *acceptance criteria* (decision, whether to accept a proposed solution, or not).

The control in cooling rate parameter is motivated as follows: if the temperature decreases too rapidly, the optimization process may settle in the local optima, but too low cooling rate is a computationally expensive, since SA requires more TS evaluations to converge. Among deterministic approaches, researchers mainly distinguish linear, exponential, proportional, logarithmic and geometrical cooling schedules. In contrast to deterministic approaches, in [64] the authors proposed an adaptive strategy to change the cooling rate, based on the statistical information, evaluated on each optimization step. Specifically, if the statistical analysis named in research a *heat capacity* shows that the system is unlikely to be trapped in the local optima, the cooling rate is increased. On the contrary, it is decreased if the possibility of being trapped is high.

In [49] the authors propose an adaptation of another hyper-parameter: acceptance criteria. The utilized mechanism is based on thermodynamics fundamentals, such as *entropy* and *kinetic energy*. The authors suggest replacing the standard acceptance criteria (based on the current temperature and the solution quality) with the one based on the solutions entropy change evaluation.

Many researches were made to investigate, which is the best among deterministic and adaptive strategies [5, 31, 60, 80, 111]. In many cases, the authors conclude that the adaptive methods provide more robust and promising results.

### Parameter Control in Evolutionary Algorithms

While searching the parameter control examples in heuristics, one will find dozens of proposed methodologies for the evolutionary algorithms. It is arising from the fact that an idea of changing the algorithm parameters dynamically came from EAs [66]. The motivation for such a number of performed studies lays in a strong dependence of an algorithms' performance on parameter values.

The deterministic and adaptive mechanisms in EAs are extended by the 3<sup>rd</sup> type — a *self-adaptive* approach. It implies an encoding of parameter values in the solution genomes, allowing them to co-evolve with the solutions at runtime [33]. All the proposed strategies could be split into two families: one includes the algorithms proposing to adapt a concrete parameter solely and the other, which includes the approaches to control a group of parameters. In EAs the commonly implicated hyper-parameters are *population size*, *selection strategies* and *variation aspects* (namely crossover and mutation operators). In case of interest, we propose the reader to analyze recently conducted reviews and researches dedicated to parameter control in evolutionary algorithms [1, 33, 66, 106].

There is one rather intriguing parameter control approach proposed for the evolutionary algorithms. In [65] the authors introduce a reinforcement learning (RL) parameter controller, whose goal is to select the EA parameters online evaluating a set of simple observables. They include: a genotype diversity, a phenotype diversity, a fitness standard deviation, a fitness improvement and a stagnation counter. The RL in this work adheres the following **MAPE-K** methodology [20]. On each iteration the observables are **M**onitored, their values are **A**nalyzed to build a parameter control **P**lan, which is **E**xecuted in the

next iteration. The letter **K** denotes a central part of this methodology — the knowledge. This set of proposed observables could be split into two logical groups. One is the algorithm-specific with the genotype/phenotype diversities and the fitness standard deviation, while the other is algorithm-independent and includes the fitness improvement and the stagnation counter. We believe the proposed RL approach could be applied to other algorithms, with the only requirement in exposing the observable knowledge. The proposed in [65] parameter control methodology may be one of the first to generalize a parameter control techniques and later in Section 3.1 we use it as a part of our approach.

### 2.3.4 Conclusion on Parameter Setting

At this point, we finalize our review of the parameter settings problems with three conclusions:

1. The parameter tuning area is investigated widely and nowadays the research settles in the form of combining different learning models to implement the SMBO algorithms in framework-like tuning systems.
2. The parameter control is actively driven by two motivations. Firstly, the runtime changes in solving process are unpredictable; therefore, the control is believed to better fit them, comparing to the statically defined by parameter tuning techniques. Secondly, the resources spent for offline parameter settings are high, but they are paid-off by a high quality of algorithm configuration. Therefore, from this perspective, the control approaches are trying to reach the quality of the offline settings, spending fewer resources. Unfortunately, nowadays the online approach is not generic to be commonly applicable.
3. The decision on concrete technique is use-case specific and is driven by the amount of available resources and the required setting quality as well.

## 2.4 Combined Algorithm Selection and Hyper-Parameter Tuning Problem

The goals of automatic machine learning are quite similar to persecuted by hyper-heuristics. They both operate on search space of algorithms (or their building blocks), which later are combined, with an objective to find the best performing ones, and used to solve the problem at hand.

In this section we review one particular representative of automatic machine learning systems. Based on the ML framework Scikit-learn [91], Auto-sklearn system [44] operates over a number of classifiers, data and features preprocessing methods **including their hyper-parameters** to construct, for provided dataset, the best performing (in terms of classification accuracy) machine learning pipeline. This problem was formalized as *combined algorithm selection and hyper-parameter tuning problem* (CASH) and presented previously in Auto-WEKA [112] system. Intuitively, it could be rephrased as follows: “For a given optimization problem, find the best performing algorithm and its hyper-parameters among available and solve the problem”.

Please note, to the certain extent Auto-sklearn is similar to HHs, which use LLHs for traversing the search space and solving the OP. However, the automatic machine learning techniques operate on the completion algorithms, the results of which are evaluated at the end of their run. On the contrary, online HHs are able to evaluate the intermediate performance of low-level heuristics, since they are anytime algorithms. CASH problem seems to be a combination of problems solved by HHs and parameter tuning approaches. We also found that the architecture search problems [40] (related to neural networks) are nothing else but particular case of CASH.



Turning back to Auto-sklearn, the crucial decisions made here is the combination of offline and online learning, resulted an exceptional performance of Auto-sklearn in classification tasks.

During the offline phase, for each of available datasets published by the OpenML community [45], search of the best performing machine-learning pipeline was done using the BO technique implemented in the discussed previously SMAC framework [58]. After that, the *meta-learning* was executed to derive the meta-features for each dataset.

The resulting combination of the datasets, machine learning pipeline and meta-features were stored and later used to initialize the online phase of pipeline search. The information from the meta-learning phase is used as follows: for a given new dataset, the system derives the meta-features and selects some portion of created during the offline phase pipelines that are the nearest in terms of meta-feature space. Then, these pipelines are evaluated on a new dataset to initialize the BO in SMAC. This decision results in the ability to evaluate well-performing configurations at the beginning of the tuning process.

During the online phase, another crucial improvement was introduced. Usually, while searching the best-performing pipeline, a lot of effort is spent in order to build, train and evaluate intermediate pipelines. After each evaluation, only the results and the pipeline description are stored, but the pipeline itself is discarded. In Auto-sklearn, however, the idea lays in preserving previously instantiated and trained pipelines, obtained while solving the CASH problem. Later, they are used to form an ensemble of models and tackle the problem at hand together. This means that the results of this architecture search are a set of models with different hyper-parameters and preprocessing techniques, rather than a single model. This ensemble starts from the worst performing ones (obtained at the beginning of the search) and ends with the best suited model for the respective dataset. Naturally, each ensemble members' influence on the final results is weighted.

The potential of offline phase is derived entirely from the existence of such a dataset repository and depends on the availability of homogeneous datasets. The proposed online methodology, which mimics the regression trees, is more universal and could be reused widely.

In general, an empirical investigation of Auto-sklearns' universality would be rather intriguing, since the only cases of Auto-sklearn application we managed to find are the classification tasks but not regression problems [13, 44].

The field of automated machine learning is one of trending research directions, that is why there exist dozens of open-source systems, such as *Auto-Weka* [112], *Hyperopt-Sklearn* [71], *Auto-Sklearn* [44], *TPOT* [88], *Auto-Keras* [61], etc. Among open-source, there are many commercial systems, such as *RapidMiner*, *DataRobot*, Microsoft's *Azure Machine Learning*, Google's *Cloud AutoML*, and Amazon's *Machine Learning on AWS*.

## 2.5 Conclusion on Background and Related Work Analysis

In this chapter we have presented the review of optimization problems, their concrete instances and existing solver types focusing on the heuristics. There exist several levels of generality in heuristic solvers: simple heuristics, meta-heuristics and hyper-heuristics.

The applicability of each algorithm is problem-dependent and derives from the exploration-exploitation balance and strength, revealed in a particular case. It is difficult to guess beforehand, which heuristic will outperform the others in an unforeseen use-case. With respect to this, hyper-heuristics seems to be the most perspective and universal solvers, since they do not tackle the problem directly, but rather select and apply the best suited among controlled algorithms.

From the other perspective, the solver performance is also dependent on the values of its parameters. It turns out, that the parameter setting is also an optimization problem. There exist several ways to solve it: (1) set the values manually, based on experience and intuition, (2) utilize the parameter tuning



systems, which find the best values automatically and later use those found parameters, or (3) exploit the parameter control mechanisms. Among all strategies, the last seems to be the happy medium, since tuning requires lots of expensive algorithm executions to produce good parameter settings, while manually choosing hyper-parameters is an error-prone process that requires experienced guidance. The analysis of parameter control approaches showed that the existing techniques are heuristic-dependent, therefore, our first research question is defined as follows **RQ1** *Is it possible to perform the algorithm configuration at runtime on a generic level?*

The outcome of no-free-lunch theorem cannot be ignored, according to which no single algorithm can tolerate a broad range of problems equally outperforming other solvers. That is why we cannot set aside hyper-heuristics, which are designed to find the best solving algorithm suited for a particular optimization problem case.

The research in automatic machine learning has made a step further and tends to combine both algorithm selection and parameter tuning problems into a single CASH problem, formalized in [112]. The search space in CASH problem is formed of algorithm variants and their respective hyper-parameters. However, one solver cannot use the parameters of another, thus, the resulting search space happens to be ‘sparse’. In general, the structure of CASH problem is almost the same as regular parameter tuning case. That is why the commonly used solvers for CASH problems are the parameter tuning systems: SMAC in Auto-sklearn and Auto-Weka, Hyperopt in Hyperopt-Sklearn and so forth. Not many surrogate models are able to handle the sparse search spaces: random forest machine learning model and Bayesian optimization approaches with exotic kernel density estimators [75]. Even fewer optimizers are able to perform well in such sparse spaces. The other drawback is that the CASH problem definition is limited to searching the algorithm and its parameters in an offline manner.

We believe that the solutions of both algorithm selection and parameter setting problems is highly dependent on a problem at hand. That is why a search for the best tool (solver) and its setting (parameters) should be performed in an online manner, in other words, while solving the optimization problem. Since the generic parameter control concept was not proposed yet, naturally, we were not able to find the techniques to merge and solve both the algorithm selection and parameter control problems in runtime. Therefore, we defined our second research question **RQ2** *Is it possible to simultaneously perform algorithm selection and parameters adaptation while solving an optimization problem?*

As CASH merges algorithm selection and parameter tuning techniques to get the outstanding performance, we found a merge of online algorithm selection and parameter control an intriguing and worth-to-try idea. However, the amount of spent resources and the imprecision of surrogates estimations for simultaneous search of both the algorithm type and its parameter values may be discouraging. To explicitly evaluate this, we define the final research question as **RQ3** *What is the effect of selecting and adapting algorithms while solving an optimization problem?*

#### **Research objective defined.**

In this thesis we are trying to achieve the best of both online algorithm selection and parameter control worlds. The resulting approach should be able to solve an optimization problem, applying *the best suited low-level-heuristic and setting its parameters at runtime*. With this idea in mind, we investigate a possibility of turning existing parameter tuning system into an **online selection hyper-heuristic with parameter control in low level heuristics**.



## 3 Online Selection Hyper-Heuristic with Generic Parameter Control

While there exists no universal approach to control the parameters of the algorithm (Section 2.3.4), our conclusion was that there exists no approach to combine both online techniques for the algorithm selection and the parameter settings (Section 2.5).

In this Chapter we propose the approach to solve this problem, excluding the implementation details. In Section 3.1, we introduce a generic parameter control technique and expand it with the process of algorithm selection. As concluded in Section 2.5, the main weakness of the reviewed approaches to tackle CASH problems lays in the inability of learning mechanisms to fit and predict in sparse search spaces. The same issue arises in case of online algorithm selection and parameter settings, and we solve it on two levels: 1) in the search space structure and 2) in the prediction process. In Section 3.2 we present a joint search space of both algorithm selection and parameter control problems. We outline functional requirements for such search space. Next, we describe a related prediction process in Section 3.3. We decouple the learning models from the search space structure and provide a certain level of flexibility in the usage of different learning models. Finally, in Section 3.4 we direct our attention to the low-level heuristics (LLH) — workhorses of our approach. We highlight the requirements to LLH that are crucial within the scope of this thesis.

### 3.1 Combined Parameter Control and Algorithm Selection Problem

The basic idea of parameter control approaches lay in the solver behavior adaptation as the response to changes in the solving process (Section 2.3.3). As we mentioned in the heuristics review (Section 2.2), the algorithm performance is highly dependent on the provided exploration-exploitation balance, which in turn, depends on (1) the algorithm itself and (2) its configuration. The task of parameter control is to find such parameters, which provide the best performance.

In our work, we solve the parameter control problem by utilizing an approach for evolutionary algorithms similar to the one proposed in [65] reinforcement learning (RL). The underlying idea of RL could be described as a process of performing actions in some environment in order to maximize the reward obtained after each performed action. To apply this technique to the parameter control problem, we should define what those *actions* are and how to estimate the *reward*. Therefore, in order to make the parameter control applicable to a broad range of algorithms, we analyze not the solver state itself but the optimization process (in [65], the authors use both algorithm-dependent and generic metrics). To realize the MAPE-K control loop, we should interrupt the solver, analyze the intermediate results, learn the current trend among parameters, configure the solver with the most promising parameter values and continue solving. The number of MAPE-K loop iterations  $i$  define the granularity of learning, where one should balance between *time to control* (TTC) the parameters vs *time to solve* (TTS) the problem. Naturally, the limitation of proposed approach is  $TTS \gg TTC$ , therefore, we are restricted to use-cases with large TTS w.r.t. TTC.

To evaluate the gained in iteration  $i$  reward, instead of using the solution quality straightforwardly, we calculate the *quality improvement*, obtained with the configuration  $C_i$ . When the search process

converges towards the global optimum, the improvement value tends to decrease, since the amount of significantly better solutions drops. Using the improvement values directly could confuse the learning models and, therefore, cause the prediction quality to struggle. To solve this issue, the relative improvement (RI) of solution quality is calculated:

$$RI = \frac{S_{i-1} - S_i}{S_{i-1}} \quad (3.1)$$

In Equation (3.1)  $S_{i-1}$  and  $S_i$  are the solution qualities before and after  $i^{th}$  iteration respectively.

The evaluated  $C_i \rightarrow RI$  pairs in previous iterations are then used to predict a configuration for the next iteration  $C_{i+1}$ . Please note, here we utilize the notion of *sliding learning window* to follow a possibly changing trends of the optimization process, therefore, we use only N (pcs., or %) of the latest available  $C_i \rightarrow RI$  pairs. Moreover, we made two other decisions for the sampling process: (1) hide the search space shape and (2) use the surrogate models for finding configurations that lead to the highest RI. After sampling the  $C_{i+1}$  configuration, we set it as the solvers' parameters. To proceed with the solving process, we initiate the solver with the solutions obtained at  $i - 1$  iteration as well.

When it comes to the algorithm selection problem (discussed in Section 2.2.5), we treat the solver type itself as a subject of parameter control and use the proposed RL approach to estimate the best performing algorithm. However, when we add the solver type as a parameter, the resulting search space becomes sparse and requires a special treatment. There exist two commonly used approaches to tackle this problem. The first [41, 58, 93] requires a special type of learning models, while the second [79] suggests the problem transformation in a way of excluding the undesired characteristics. During the review of model-based parameter tuning approaches (Section 2.3.1), we made a conclusion that most of the reviewed systems follow strictly the first idea. For instance, the surrogate models in BOHB [41] and BRISE [93] use the Bayesian probability density models. Those surrogates could naturally fit the sparse search spaces (described in the following section), but the proposed approaches are not able to make the predictions effectively, since most of predicted configurations will violate the dependencies. As an example, let us imagine after  $i^{th}$  iteration, the surrogate models learn about two superior parameters: one indicates a well-performing heuristic type (genetic algorithm), the other — an effective configuration for another algorithm type (an exponential cooling rate for simulated annealing). In this case, the reviewed systems sampling methods will tend to predict invalid configurations with those two parameter values.

In this thesis we adapt the second approach of problem transformation used in [79] for sampling the valid configurations only. The following section depicts a required preparation step made in the search space, while Section 3.3 is dedicated to the prediction process.

## 3.2 Search Space Structure

When time comes to selecting not only the solver parameters but also the solver itself, the united search space can no longer be presented as a 'flat' set of parameters, since it tends to produce many invalid parameter combinations. Let us estimate the number of all possible configurations in comparison to the proportion of meaningful ones. Suppose we have  $N_s$  solvers, each exposing  $N_{s,p}$  hyper-parameters with  $N_{s,p,v}$  possible values. The aggregated quantity of configurations  $N_c$  in the disjoint search spaces is calculated as a number of possible combinations using Equation (3.2).

$$N_c = N_s \cdot \prod_1^{N_{s,p}} N_{s,p,v} \quad (3.2)$$

However, if we decide to tune (or rather to control) the solver type itself, the resulting quantity of possible configurations is calculated using Equation (3.3).

$$N_c = \prod_{s=1}^{N_s} \prod_{p=1}^{N_{s,p}} N_{s,p,v} \quad (3.3)$$

For the better intuition, let us try some numbers. By setting all  $N_s = N_{s,p} = N_{s,p,v} = 3$  (a rather small example), the number of configurations estimated separately for each solver equals to  $N_c = 81$  (Equation (3.2)). However, if we join the parameter spaces of all three solvers, Equation (3.3) shows a significant growth in the search space size:  $N_c = 19683$ . Please note, the number of *unique and valid* configurations remains the same; thus, in the joint space it is only  $\approx 0.4\%$ . By setting the  $N_s = N_{s,p} = N_{s,p,v} = 4$ , this number drops to  $\approx 9 \cdot 10^{-8}\%$ . It could decrease even further, if the dependencies among hyper-parameters exist. In such case, the predictive abilities of models may struggle.

To overcome this problem, we utilize a certain idea, similar to the one used in IRACE [79]: *explicitly indicate the dependencies as parent-child relationships among the search space entities, firstly predicting the parent parameter, and the children parameter afterwards*. This gives us an opportunity to treat the algorithm type as a regular categorical parameter, making the search space structure uniform and simplifying the prediction process.

This decision sets the following search space *structural requirements* (S.R.):

- S.R.1 The **parent-child relationship** must describe dependencies between different parameter types.
- S.R.2 The **uniform parameter type** simplifies the structure and hides the domain-specific intent of each parameter; therefore, algorithm type and its hyper-parameters are treated in the same way.
- S.R.3 The **value-specific dependencies** describe certain parent value(s), when the child should be exposed. For instance, the parameter *algorithm type* has a number of possible values, each requiring its own set of hyper-parameters, which should remain hidden for the other solver types.

Figure 3.1 shows an example of such a search space with  $s$  algorithm types, each having  $p$  parameters with  $v$  possible values. The entities with triangles  $\nabla$ , namely, the concrete values of parameters, form the joint-points to which the other parameters could be linked.

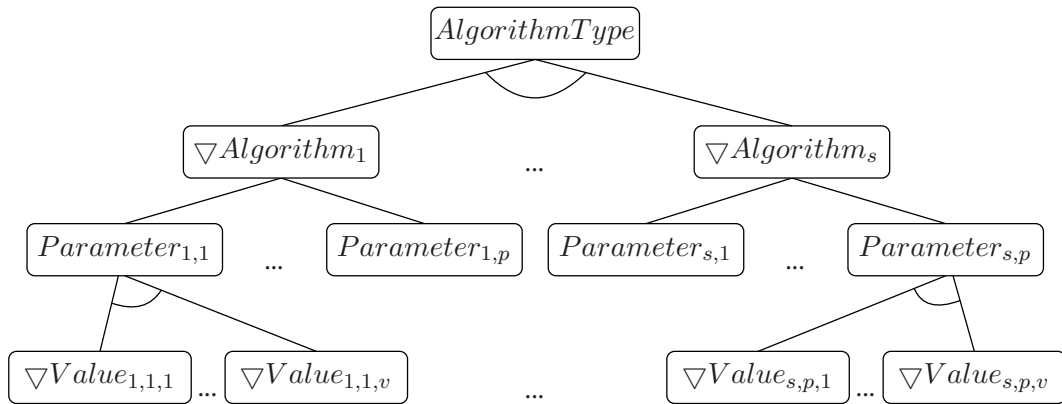
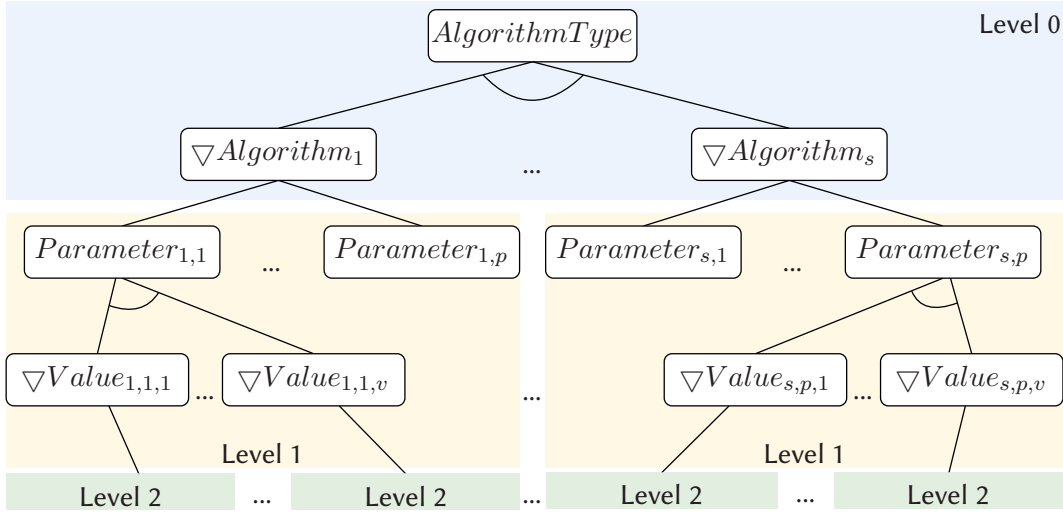


Figure 3.1 Search space representation.

### 3.3 Parameter Prediction Process

After formalizing the search space structural requirements, let us switch to the prediction process and define the *functional requirements* for both search space and prediction process, which should be fulfilled to decouple the learning models from the complex search space shape.

The idea of this decoupling lays in resolving the value-specific dependencies among the parameters in a step-wise prediction approach. To do so, we firstly predict the parent value, which in case of the hyper-heuristic is a low-level heuristic type (Level 0 in Figure 3.2). Afterwards, the search space must expose the parameters of this solver only, ignoring the others (Level 1 in Figure 3.2). The dependencies among exposed parameters are then handled in the same way (Level 2 and further in Figure 3.2).



**Figure 3.2** Level-wise prediction process.

The prediction on each level is performed in three main steps: (1) filtering the required for this level information, (2) building the surrogate model and (3) finding the best performing parameters on this level.

While building the surrogates and making the predictions, we ignore the information from levels above and below with the motivation to simplify the overall process and hide the search space structure. In addition, when we predict on the parent level, it will not change on the descendant levels, therefore, we do not need to operate useless static information. While the backward ignorance is clear, the forward data omission puts a restriction on the surrogate models. Cutting off the parameter values from the deeper levels, we may get the data points with the same parameter values for current level (also named *features* in machine learning) but different results (*labels*). Thus, only those surrogate models should be used on such level(s), which will not be confused by the multi-valued dependencies in data (when the same input results in different outputs). In the implementation description in Section 4.3.3 we clarify, which models are the better choice in such cases and implement one of the promising.

Certainly, while solving the problem, the quality trends among parameter values may change. For instance, at later stages the domination of one solver could be declined in comparison to others. Or else, the previously best-performing parameter values are not good enough and should be replaced by the other. These changes may be caused by the variety of reasons, which we are not tackling. Instead, the old trends should be left out by some forgetting mechanism.



At this point, let us summarize the functional requirements for the search space (S.F.R) and prediction process (P.F.R).

- **In the search space we need:**

- S.F.R.1 The **data filtering mechanism**, which will be used to find out only those feature-label pairs, which can be utilized to learn the dependencies on current level.
- S.F.R.2 The **sampling propagation mechanism**, which will be used to randomly sample the parameter values for the next level taking into account currently available parameter values, which is required to expose the parameters after predicting on current level.
- S.F.R.3 The **parameter description mechanism**, which will provide the information about a type and possible values for the given parameters. This knowledge will later be used by the models for making the parameters' values prediction.
- S.F.R.4 The **configuration validation mechanism**, which will find out, whether the parameter ranges are not violated by the selected values (flat validation), and whether for all selected values the dependent (exposed) parameters are selected properly as well (deep validation).

- **In the prediction models:**

- P.F.R.1 The **model encapsulation mechanism**, which should aggregate and hide the level-wise approach of the search space traversal and the feature ignorance as well. On the contrary, it should rely on underlying models for making the prediction.
- P.F.R.2 The **model unification mechanism**, which is required for the system variability in terms of the learning and sampling algorithms.
- P.F.R.3 The **information forgetting mechanism**, which is required to follow only the recent trends among the parameter values dependencies.

### 3.4 Low-Level Heuristics

As we stated in Section 2.2.5, hyper-heuristics are built of two main components — the high-level heuristic (HLH) and the low-level heuristic (LLH). Please note, the used *solver type* term in this chapter is nothing else but the LLH in hyper-heuristic. The previous two sections were dedicated to the search space and prediction models description, which form the logical components of the HLH. No hyper-heuristic could work without LLH, therefore, in this section we discuss the requirements for the low-level heuristics.

The proposed idea of the MAPE-K reinforcement learning application implies the usage of anytime algorithms (see classification of solvers in Section 2.1.2). They may be implemented in various frameworks or even programming languages, the only requirement is to expose a common interface.

Firstly, we want these algorithms to continue their solving process from the previously found solution but not to start the process from scratch. Before the start, they should accept the predicted by HLH hyper-parameters, and the previously reached solution(s) (possibly, by the other solver).

Secondly, after the algorithm execution, the solution quality should be estimated and reported to the HLH to proceed with the RL.

Both actions should be performed in the implementation-independent way, therefore, following a pre-defined shared interface described above. We discuss it in Section 4.4, dedicated to LLH implementation.

### 3.5 Conclusion of Concept

When the requirements, specified for the search space and the prediction process are fulfilled, it provides a certain level of overall system flexibility in the following use-cases:

1. The **parameter tuning** case is possible, if one builds a search space of the single LLH, its hyper-parameters, and disables the solution transfer between the iterations.
2. The **parameter control** case is possible, if one builds a search space of the single LLH, its hyper-parameters, and enables the solution transfer between the iterations.
3. The **offline selection hyper-heuristic** is possible, if one builds a search space of the multiple LLHs, and disables the solution transfer between iterations. In this case, the LLHs will be used with the static hyper-parameters.
4. The **online selection hyper-heuristic** is possible, if one builds a search space of the multiple LLHs, and enables the solution transfer between iterations. In this case, the LLHs will be used with the static hyper-parameters as well, but initialized with the obtained in previous external iteration solutions.
5. The **online selection hyper-heuristic with parameter control** is possible by building the search space of multiple LLHs, their hyper-parameters and enabling the solution transfer between iterations.

Please note that the offline cases estimate the solution quality directly, while the online cases use the relative solution quality improvement.

It is worth mentioning that the proposed structure of search space representation is similar to the *feature model*, used to describe the software product lines (SPL) [104]. In Figure 3.1 and Figure 3.2 we used the notions from SPL feature models to denote *alternative* parameter values. The process of configuration construction within a search space can be treated as the *staged configuration* in SPL.

## 4 Implementation Details

In this Chapter we dive into the development description of listed in Chapter 3 requirements.

The best practice in software engineering relies on an implementation effort minimization with the help of already existing and well-tested code reuse. With this idea in mind, we select one of the reviewed in Section 2.3.1 open-source parameter tuning frameworks as the code basis for the desired RL-based hyper-heuristic. We also reuse the low-level heuristics (LLH) implementation from other meta-heuristics frameworks. The LLH basis may be used almost out-of-box, but the HLH basis requires changes to utilize the reinforcement learning approaches.

In Section 4.1 we analyze the parameter tuning frameworks from a perspective of required adaptation effort to implement listed in Section 3.3 HLH characteristics. We conclude the analysis selecting the best-suited HLH code basis in Section 4.1.2. Afterwards, we split the HLH adaptation process on two similar to presented during the concept description logical parts: in Section 4.2 we discuss the search space development, while Section 4.3 is dedicated to the prediction process. Finally, in Section 4.4 we perform a code basis selection for LLH, present a set of reused meta-heuristics, their adaptations and the importing process into our hyper-heuristic.

### 4.1 Hyper-Heuristics Code Base Selection

To begin with the analysis of frameworks, we outline important characteristics from the implementation perspective.

The first two crucial criteria are *variability* and *extensibility* of framework. Since we are planning to use a possibly (but not obligatory) different models for the LLH selection and parameters control, the code basis should be variable in terms of models usage for each prediction level (see Figure 3.2). The desired HH and specifically HLH should be easily extensible in terms of not only the surrogate models, but also other features such as termination criteria, information filtering, data preprocessing and so forth.

The next criterion is the support for *online optimization*. It is a slightly complex system characteristic, which we are willing to distinguish. As it turns out, many parameter tuning systems require full evaluation of target system, others expose early termination mechanisms, but all of them are forcing TS to start solving the problem at hand each time from scratch. In the case of our hyper-heuristic, we treat the LLH configuration evaluation as a trial to improve the problem solution results. It implies an important LLH ability to tackle the (OP) using reinforcement learning approaches (Section 3.1).

The final characteristic is the *conditional parameters* support. This complex feature influence on not only the search space representation mechanisms, but also the prediction process. Therefore, we pay a close attention to both of them from the conditional parameters support perspective.

#### 4.1.1 Parameter Tuning Frameworks Analysis

**SMACv3** We begin our review with the implementation of Sequential Model-based Algorithm Configuration framework, distributed under the BSD-3 license. The idea of SMACv3 lays in an enhancement of the ROAR mechanism with a model-based sampling algorithm. ROAR is a derivative from the FocusedILS

algorithm (solver in the parameter tuning framework ParamILS [59]), where each evaluation of a new solution candidate on a problem instance was performed sequentially and in isolation. Therefore, since the ROAR evaluation strategy is also used in SMACv3, we have found that it requires a considerable effort to synchronize the progress between different runs for the online problem-solving.

As we have mentioned in Section 2.3.2, the underlying surrogate model in SMACv3 is selected statically among random forest or Gaussian process kernel density estimator. Both models could fit to complex dependencies among parameters. In the next configuration sampling process the *one-exchange* neighborhood of the best found so far configuration is traversed using the created surrogate model and the expected improvement estimations. The ability of both surrogates to fit a sparse search space is promising, and the usage of expected improvement guarantees to converge the search process to the global optimum given enough time. However, the major drawback in this system is a lack of abilities to include the conditional dependencies between parameters into the sampling process. Since, to the best of our knowledge, the one-exchange neighborhood is unaware of the dependencies, it violates them while sampling and results in illegal parameter values combinations. Those cases are naturally controlled and rejected by the search space representation framework ConfigSpace [78], but we believe in case of sparse search spaces it could lead to ineffective sampling and system predictive abilities struggling. Unfortunately, we did not find any officially published empirical studies of such cases and could only make guesses based on own intuition, but the advises of SMACv3 developers for such use-cases<sup>1</sup> may serve as evidence to the correctness of our assumptions. One of the possible solutions here can be the implementation from scratch of a conditional-aware one-exchange neighborhood definition and for sampling process, which requires much implementation effort.

**IRACE** This framework implements the iterated racing algorithm to evaluate a set of configurations during the parameter tuning session (Section 2.3.2). The software is distributed under the GNU General Public License with an open source code.

The framework uses a *Friedman test* [28], or *paired t-test* as an alternative for statistical analysis of racing in parallel configurations. As the surrogate models, IRACE uses the probability distributions of those parameter values, which proved to be good during the racing step. The configuration prediction process is defined as a step-wise sampling on previously constructed distributions. It elegantly handles the conditions among parameters and illuminates a possibility of invalid configuration appearance. Unfortunately, this solution is static in terms of variability and extensibility on the learning mechanisms.

From the perspective of parallel evaluations, the framework utilizes all available resources at the beginning of each racing step, but as the process continues, fewer evaluations are executed simultaneously, therefore, part of available resources is idling and not utilized completely at all stages of IRACE execution.

For the online problem solving support, let us discuss the racing algorithm. As mentioned in Section 2.3.2, this step is executed on (1) a set of TS configurations sampled for evaluation and (2) a benchmark set of optimization problems. Multiple instances of TS are initializing with the provided configurations and starting to solve the problem set, while the racing algorithm terminates the worst-performing settings. In case of hyper-heuristic, it is possible to define the benchmark set as a single problem instance divided into parts of TS running time. At each pause we may perform the synchronization of current solutions to proceed with the best found results. By doing so, we adapt the system to online problem-solving cases, however, the granularity of parameter control will be reduced. The reason for such reduction is the amount of information obtained after each race: only the best configurations are reported leaving the performance evidence of others behind, but we believe this information may be used to create a more precise surrogate model.

---

<sup>1</sup>Visit SMACv3 repository <https://github.com/automl/SMAC3/issues/403>

**HpBandSter** As we discussed in Section 2.3.2, HpBandSter is an implementation of BOHB algorithm, which turns to be a hybridization of Hyperband and Bayesian optimization approaches.

A role of Hyperband in this duet is the configuration evaluation and comparison, while the Bayesian Tree Parzen Estimator (TPE) suggests which configuration to evaluate next. The idea behind this combination lays in elimination of each algorithm weak sides with strengths of the other. For instance, in original Hyperband the configuration sampling is made uniformly at random, which results in a slow converge of an optimization process. On the contrary, a drawback of BO TPE lays in a configuration evaluation process. Naive Bayesian optimization approaches do not take into account the TS performance early evidences. Thus, even when the proposed configuration results in a poor TS initial and intermediate performance, which may be an evidence of a weak final performance, BO still continues the TS execution. These facts motivated authors to merge those two algorithms and create one for parameter tuning with strong anytime (HB) and final (BO) performance. The resulting hybrid effectively uses available computational resources in parallel (HB) in combination with robust learning mechanisms (BO).

Let us discuss the process of handling the conditions between parameters. HpBandSter as well uses ConfigSpace framework for the search space representation. As we discussed during the SMACv3 review, ConfigSpace naturally allows encoding the dependencies and conditions among parameters. TPE learning models are also able to fit these dependencies by means of implemented *imputation* mechanism [75]. In short, in order to fill ‘sparse’ configurations with data, the disabled parameters are replaced with their default values. Later, while building the surrogate models those default values are ignored, therefore, the probability density estimations still represent a proper parameter values distributions. However, consider a case of two configurations families appearance:  $C_1$  and  $C_2$ , such that some parameter  $P_i$  is forbidden in  $C_1$  but required in  $C_2$ . On the contrary, another parameter  $P_j$  is required in  $C_1$  but forbidden in  $C_2$ . If these configuration families are turning to be superior, the resulting probability densities will be biased towards  $P_i$  and  $P_j$  values. As a consequence, the utilized in HpBandSter prediction mechanism will sample non-default parameter values for both  $P_i$  and  $P_j$ , which results in the configurations with violated parameter dependencies. The sparser the search space is, the more harming an effect will be in a prediction performance. The possible treatment here is to change the sampling process by an intermediate layer addition, which will perform the parameter prediction in level-wise approach suggested in Section 3.3.

**BRISv2** BRISv2 is a software product line (SPL), created with an aim at solving the expensive optimization problems in general and for the parameter tuning in particular (Section 2.3.2).

The advantage of BRISv2 over other systems comes from its *main-node* modular design. It is a set of cooperating core entities (Experiment, Search Space and Configuration) with other non-core entities, exposed to user for variability. The prediction models, termination criteria, outliers detectors, repetition strategies, etc. are representatives of these non-core and variable components. A number of implementations are provided out-of-the-box for all variable entities, but we focus our attention only on the implemented sampling process. The reason for such a greedy review is that the underlying search space representation is carried out by the same ConfigSpace. The provided surrogate models here are ridge regression model with polynomial features and Bayesian Tree Parzen Estimator (TPE). We are not going to repeat ourselves reviewing the ConfigSpace + TPE combination, but we have to put a few words about the ridge regression.

Ridge is the linear regression model with regularization [55], often used in machine learning field. Being a linear model, its abilities to fit sparse search spaces is poor and, therefore, a machine learning community suggested treating such cases with *conditional linear regression models* [24]. The underlying idea is to split the search space into sub-spaces and to build separate regression models in each of them. Unfortunately, this approach was not built-in into the ridge regression model used in BRISv2.

As for the online problem solving support, the routine of an optimization process implemented in BRISv2 is very similar to the reinforcement learning. After each new obtained evidence (configuration), a new surrogate model is built to react to the learning process by predicting the next configuration. This facilitates the implementation of problem solving with runtime system adaptations, presented in Section 3.1.

### 4.1.2 Conclusion on Code Base

Most of the reviewed parameter tuning systems share the same SMBO approach for problem solving. They utilize rather similar techniques for the surrogate models creation and predictions making, however, the different system architectures are implemented. To sum up our review, we utilize the term *quality* to aggregate both (1) provided out-of-the-box the desired characteristic support and (2) the required effort to adapt it, if necessary. For the visual representation, we collect the reviewed characteristic qualities of each software framework into Table 4.1 and quantize them into three ordinal values:

1. **Poor** quality denotes a weak characteristic support and much effort required to improve it.
2. **Average** quality indicates a weak characteristic support, which requires less amount of effort to provide it.
3. **Good** quality means a good characteristic support out-of-the-box and requires minor or no changes at all.

**Table 4.1** Code basis candidate systems analysis.

Characteristic	SMACv3	IRACE	HpBandSter	BRISv2
Variability & extensibility	Average	Poor	Average	Good
Online optimization	Average	Average	Average	Good
Conditional parameters	Poor	Good	Poor	Poor

Most of the reviewed software systems were created as an implementation of some concrete algorithm (or combination of algorithms), which results in a system flexibility reduction. Every reviewed framework requires much adaptation effort and the preparation steps should be performed in different parts of a system. Between such features as a proper support of conditional parameters and variability-extensibility, the former plays a settled role in our case. Therefore, we conclude that the BRISv2 framework is the most promising candidate for the hyper-heuristic with parameter control creation.

## 4.2 Search Space

Previously, in Section 3.2 we presented a set of structural requirements for the search space representation: parent-child relationships should be presented explicitly to allow combinations of different parameter types. For the prediction process support, in Section 3.3 we listed the functional requirements in a form of mechanisms: data filtering, sampling propagation, parameter description and configuration verification. In this section we analyze the available ConfigSpace framework, how it fits to our requirements and decide, whether to use it or to set aside in order to perform our own search space representation implementation.



### 4.2.1 Base Version Description

From the structural point of view, in ConfigSpace<sup>1</sup> the parameter coupling is made implying parent-child relationship, which fits into our requirements. The set of parameter types suite the most of use-cases and the value-specific dependencies are supported as well. Thus, the structural requirements S.R.1, S.R.2 and S.R.3 are perfectly met.

When it comes to the functional requirements, ConfigSpace samples random configurations in a completion manner. In other words, there is no step-wise process of configuration construction, but only the final and valid results are produced. To the best of our knowledge, there is no straightforward way to expose the underlying parent-child dependencies among parameters and investigate a tiered search space structure, which is required for the prediction models. As a consequence, the data filtering mechanism should be implemented on a side and the sampling propagation as well. The framework exposes an ability to validate a fully created configuration but not a partial one (flat validation). It is also worth mentioning that the used in ConfigSpace configuration is a proprietary class. As for the parameter description, the amount of exposed knowledge is satisfying. Here we conclude that the functional requirements, except S.F.R.3, are not met.

As the conclusion, we decided to set aside the 3<sup>rd</sup> party ConfigSpace framework. The reason for doing so is mostly motivated by the amount of required adaptation effort and partially by involvement of obligatory external dependencies.

### 4.2.2 Search Space Implementation

From the structural requirements we know that the parameters in search space should be treated uniformly. The desired feature tree structure is handled by the *composite* design pattern. With this idea in mind, we construct the search space as a composite *Hyperparameter* object with four possible hyper-parameter types: integer and float as a numerical parameter family, nominal and ordinal as a categorical family. This fulfills specified in Section 3.2 S.R.2.

With the code snippets provided through the explanation, we highlight the signatures of implemented methods, which fulfill specified in Chapter 3 requirements.

**Search space construction.** The S.R.3 (parent-child relationship) implementation is performed by adding a construction method *add\_child\_hyperparameter* in the *Hyperparameter* class (Listing 4.1). It should be called on a parent object, specifying the activation value(s) (*activation\_categories* argument) of parent hyper-parameter which should expose the child.

```

1 class Hyperparameter:
2     ...
3     def add_child_hyperparameter(self, other: Hyperparameter, activation_categories: Iterable[
4         CATEGORY]) -> Hyperparameter

```

**Listing 4.1** S.R.1 implementation.

**Please note**, currently we require the support of composite construction only by means of categorical parameters, therefore, *add\_child\_hyperparameter* requires a list of activation categories. We postpone an enhancement of composition on numerical ranges for future work.

**Search space role in prediction.** Imagine several configurations were evaluated and their relative improvement is already estimated. For making the prediction in a tiered approach, the parameter

<sup>1</sup>ConfigSpace GitHub repository: <https://github.com/automl/ConfigSpace>

## 4 Implementation Details

values on a current level should be selected before moving to the next one. In order to do so, we firstly filter data, which fits to this level by means of S.F.R.1. It is implemented in form of recursive hyperparameter method *are\_siblings*, presented in Listing 4.2. The filter accepts already selected parameter values and iterates over the available configurations. At each iteration it finds out, whether the already chosen parameter values (*base\_values*) form a sub-feature-tree of the target configuration parameter values (*target\_values*). For instance, if the selected LLH type in *base\_values* is not the same as one in *target\_values*, the result will be negative.

```
1 class Hyperparameter:
2     ...
3     def are_siblings(self, base_values: MutableMapping, target_values: MutableMapping) -> bool
4     ...
```

**Listing 4.2** S.F.R.1 implementation.

After data filtering, the time comes to find out the values of which parameters we must predict. In order to do so, the search space must expose those parameters by means of S.F.R.2 implemented in *generate* method with signature presented in Listing 4.3. Since we always interact with a search space root object, the call to *generate* is executed recursively. If a callee finds itself in *values* argument (which depicts the current *parameter name*  $\rightarrow$  *parameter value* mapping), it redirects a call to all *activated* children. If it does not, it adds itself a to the *values* and terminates the recursion.

```
1 class Hyperparameter:
2     ...
3     def generate(self, values: MutableMapping) -> None
4     ...
```

**Listing 4.3** S.F.R.2 implementation.

A randomly sampled for the current level values are then used to obtain the level description. It is then used to (1) cut-off the data from levels above and below (simply selecting the required key-value pairs from the parameter mapping), to (2) build the surrogate models and to (3) make the prediction of parameter values on current level.

The creation of surrogate model requires an available data (parameters) description. Thus, the S.F.R.3 implementation is performed in method *describe* with signature presented in Listing 4.4. This is once again a recursive call, which terminates, when the parameter object cannot find the activated children or himself in the provided *values*. The resulting description is a mapping from the parameter name to its type and range of possible values: either a set of categories for categorical, or lower and upper boundaries for numerical types.

```
1 class Hyperparameter:
2     ...
3     def describe(self, values: MutableMapping) -> MutableMapping[Name: [Type, Values]]
4     ...
```

**Listing 4.4** S.F.R.3 implementation.

This description is then used by the prediction models for building surrogates and making the parameter values predictions, which replace obtained after *generate* method call randomly sampled values.

The process described above is controlled by means of S.F.R.4, implemented as method *validate* (signature in Listing 4.5). The control occurs in two places. Firstly, before starting a new loop of *filter*  $\rightarrow$  *propagate*  $\rightarrow$  *describe*  $\rightarrow$  *predict* we check whether the construction process is not finished (deep validation), meaning all parameter values were chosen, and we have a valid configuration. Secondly, after making the prediction by models (flat validation), it verifies if the parameter boundaries are not

violated. In case of violation, the prediction is discarded and the randomly sampled values are used instead. Since the implemented in search space sampling process (*generate* method) guarantees to provide valid parameter values, after maximally  $N$  loops mentioned above, we derive a new and valid configuration, where  $N$  is a maximal depth in the defined search space.

```

1 class Hyperparameter:
2     ...
3     def validate(self, values: MutableMapping, recursive: bool) -> bool
4     ...

```

**Listing 4.5** S.F.R.4 implementation.

## 4.3 Prediction Process

The next step is an investigation and planning of the prediction logic adaptation. In Section 4.1.1 we learned that BRISv2 provides two learning models: Bayesian TPE and ridge linear regression. Both of them could be used as surrogates within a tiered sampling, however, this process should be generalized.

P.F.R.1 implies the addition of entity, which encapsulates the prediction process, described in Section 4.2.2. We also make this entity responsible for the forgetting strategy, therefore, reaching P.F.R.3. Both requirements are not fulfilled in BRISv2 yet, hence, we must implement them from scratch.

As for P.F.R.2, the current implementation of BRISv2 already provides some level of model unification with a required interface. However, during the implementation we found that it implies three logical steps binding: data preprocessing, surrogate models creation and surrogates optimization to predict a next configuration.

The following parts of this Section are dedicated to (1) P.F.R.1 and P.F.R.3 implementation in form of *Predictor* entity, P.F.R.2 fulfillment in form of the data preprocessing mechanisms decoupling from the prediction models. Please note, we postpone the implementation of an elegant surrogate optimization mechanism for future work. Instead, we utilize a simple random search over the surrogate models, since as mentioned in Section 2.3.1, given enough evaluations the random search results become comparable to model-based algorithms. Due to a cheap cost of configuration evaluation on surrogate models, we are allowed to do so.

### 4.3.1 Predictor Entity

In addition to presented logic during the search space description, a role of predictor also lays in decoupling of the learning models from: (1) feature-tree search space shape, (2) other core entities such as Configuration. Besides the static search space, the input for predictor is available at the moment data (evaluated configurations), while the desired output is a configuration. Listing 4.6 provides a pseudo-code of the predictor implementation.

To implement the information forgetting mechanism, we utilize the similar idea of *sliding window*, used in hyper-heuristics [42]. According to it, the predictor should use a specific number of the latest configurations as information for surrogate models creation. We modify this logic, allowing user to specify not only a static number, but also a percentage of the latest configurations (line 4). It fulfills the P.F.R.3. Naturally, more exotic approaches may arise such as a statistical analysis of diversification or the other types of meta-learning, but we leave it for the future work.

The next step is a prediction models decoupling from the search space structure by means of fulfilling P.F.R.1. As discussed in Section 4.2.2, to predict parameter values on each level, the models should be built on only related to this level information. For this, after filtering the data (Listing 4.6, line 11), predictor propagates the sampling from a previous level to current (line 14) and derives a description for

## 4 Implementation Details

the obtained parameters on current level (line 17-18). Independently, it instantiates a specified in settings surrogate model for this level and fits it with the obtained information (lines 21-23). Afterwards, it requests a prediction from the model (will be discussed later) and forwards the prediction for validation by the search space entity (lines 27-28). If either the model cannot properly fit the data, or the prediction is invalid, we keep the sampled randomly parameter values (lines 29-31).

```
1 class Predictor:
2     def predict(measured_configurations):
3         # Filter data according to sliding learning window
4         level_configurations = trim_in_window(measured_configurations)
5         prediction = Mapping()
6
7         # Continue prediction until get a valid configuration (Deep validation)
8         while not search_space.validate(prediction, recursive=True):
9
10            # Filtering the data for current level
11            level_configurations = filter(search_space.are_siblings(prediction, x), level_configurations)
12
13            # Propagate the prediction
14            randomly_generated = search_space.generate(prediction)
15
16            # Derive the level description
17            full_description = search_space.describe(randomly_generated)
18            level_description = trim_previous_levels(description, prediction)
19
20            # Cut-off data and build model
21            data = trim_accodring_to_description(level_configurations, level_description)
22            model = get_current_level_model()
23            model.build(data, level_description)
24
25            # Predict current level and validate prediction (flat validation)
26            if model.is_built():
27                level_prediction = model.predict()
28                if not search_space.validate(level_prediction, recursive=False):
29                    level_prediction = randomly_generated
30            else:
31                level_prediction = randomly_generated
32
33            return Configuration(prediction)
```

**Listing 4.6** P.F.R.1 + P.F.R.3 implementation pseudo-code.

For the sake of simplicity, we omit some minor implementation details and provide the description of the data preprocessing and available surrogate models below.

### 4.3.2 Data Preprocessing

The data preprocessing concepts may be split into two complementary parts: an obligatory data encoding and optional data transformation. The first is required to make the underlying model compatible with the provided data. Imagine the parameters values to be simple strings. Having a surrogate model, which is constructed as the parameter values probability densities (TPE), one should derive a numerical data by encoding those string values into numbers. The second concept is applied on data, which is already suitable. This is usually done to improve an available surrogate model accuracy by reducing the bias (learning complex dependencies in data), variance (generalization to the unforeseen data) or both. An encoding example could be simple indexing of all possible string values. It is performed

as a replacement of strings by their indexes during the data preprocessing. On the contrary, for the transformation one may try to add the polynomial degrees of available features with an aim to disclose more complex dependencies. The decision on encoding type is often defined by the learning model. In contrast, the decision on data transformation is carried out by the user and depends on the concrete use-case and experience.

All reviewed in Section 2.3.2 parameter tuning systems implement the data preprocessing only by means of an obligatory encoding and omitting the possible data transformation. In most cases it is implemented as a simple label enumeration and is not encapsulated at all (as an example, check ConfigSpaces' Configuration method `get_array`<sup>1</sup>). Being the most straightforward approach, this encoding may introduce non-existing patterns in categorical data. For instance, having 3 possible LLH types: genetic algorithm, simulated annealing and evolution strategy, it will encode such parameter values to numbers 0, 1 and 2 respectively. When such encoded data is passed to the surrogates for learning, some models may interpret it as follows: in the search space, GA could be closer to SA than ES, the distances from SA to two others algorithms are equal within a search space. To prevent this, the other type of preprocessing should be used, for instance, binary encoding.

In any case, the intent of this discussion is to provide an insight of data preprocessing importance for the reader, but the discussion of possible causes and their influence is out of this thesis scope. Here we decided to gain a certain level of flexibility by providing a uniformed wrapper for the preprocessing routines implemented in Scikit-learn machine learning framework [91]. We omit the details of wrapper implementation since it is a single object decorator, instantiated with the provided preprocessing unit. The wrapper is executed each time before the actual surrogate performs learning and after making the prediction to inverse the transformation.

To make the models and data preprocessing units interfaces compatible, we store the data in form of DataFrames — tabular data representation carried by Pandas framework <sup>2</sup>. In Listing 4.6, line 21 denotes a step of configuration objects transformation to DataFrame, keeping only the current level features.

### 4.3.3 Prediction Models

As a derivative of predictor implementation, the underlying prediction models should expose a unified interface and behavior. Due to tiered prediction process, the surrogate models are acting on the search space levels without forbidding dependencies. This enables us to use in addition to previously discussed surrogates a vast range of other learning algorithms, for instance, linear regression models. In fact, a previously used in BRISEx2 ridge regression with polynomial features is nothing else, but a combination of data preprocessing step with the ridge regression model from Scikit-learn framework. Later in this Section we discuss an implementation of a unified wrapper for Scikit-learn linear models.

As a step further, we also add the implementation of multi-armed bandit (MAB): a selection strategy proposed in [4]. It is motivated by a promising performance of the reviewed in [4] selection hyper-heuristics built on MAB. Please note, MAB is applicable only to categorical parameters types.

We also decouple the previously available in BRISEx2 Bayesian TPE from the data preprocessing logic, however, no other major changes except refactoring are required. Thus, there is no reason for the detained TPE implementation discussion here.

### Scikit-learn Linear Model Wrapper

Scikit-learn is one of the most popular open-source machine learning frameworks. As a consequence of flexible architecture, Scikit-learn often plays a central role in other products providing implementations

<sup>1</sup>ConfigSpace documentation <https://automl.github.io/ConfigSpace/master/API-Doc.html>

<sup>2</sup>Pandas Github repository <https://github.com/pandas-dev/pandas>

of numerous building blocks for machine learning pipelines. This advantage in combination with a comprehensive documentation resulted to a large and active framework community<sup>1</sup>.

All available in Scikit-learn linear regressors implement the same interface and usage routines. For instance, before making a prediction, the regression model should be trained on preprocessed data, providing *features* and *labels*. Afterwards, one may use model to make a prediction for unforeseen features and the surrogate will produce a corresponding label according to the learned dependencies. This implies that for finding the best parameter combination, one should still solve the original optimization problem but with the reduced evaluation cost.

To reuse the available in framework surrogate models, we create the wrapper as an object decorator, implementing the required in *Predictor Model* interface. The pseudo-code of this wrapper is presented in Listing 4.7.

During the model creation, we firstly instantiate features and labels preprocessors, and transform the input data (lines 4-6). The creation process includes also a model accuracy verification step, which is performed by means of cross-validation: splitting the set of data into  $k$  disjoint folds, training  $k$  model each time excluding one fold for accuracy verification (line 9). If the potential model average accuracy is less than a predefined threshold, the model is considered to be not precise enough and, therefore, rejected (line 15), forcing the predictor to use random parameter values. However, if the model is able to perform well, we train it on an entire dataset and store it for further usage (lines 12-13).

Later, for making the prediction by means of random search (if the model was built successfully), we firstly sample parameter values of this level uniformly at random (line 20). Afterwards, we transform them using the same preprocessors, applied during the model construction (line 21). Then, we make a prediction for randomly sampled features using the surrogate model and transform those predictions back into original labels (lines 23-24). Finally, we select the best features (encoded parameter values) by means of the predicted labels, reverse it transformation and return to *Predictor* (lines 27-28).

---

<sup>1</sup>Scikit-learn GitHub repository <https://github.com/scikit-learn/scikit-learn>



```

1 class SklearnModelWrapper(Model):
2     def build_model(features, labels, features_description):
3         # Execute data preprocessing
4         features_preprocessors, labels_preprocessors = build_preprocessors()
5         transformed_features = features_preprocessors.transform(features)
6         transformed_labels = labels_preprocessors.transform(labels)
7
8         # Build model and check its accuracy
9         accuracy = cross_validation(model, transformed_features, transformed_labels)
10        if accuracy > threshold:
11            # Training on all available data
12            model.fit(transformed_features, transformed_labels)
13            model_is_built = True
14        else:
15            model_is_built = False
16        return model_is_built
17
18    def predict():
19        # Solving surrogates optimization problem by means of random search
20        features = random_sample(features_description)
21        features_transformed = features_preprocessors.transform(features)
22
23        labels_predicted_transformed = model.predict(features_transformed)
24        labels_predicted = labels_preprocessors.inverse_transform(labels_predicted_transformed)
25
26        # Select those parameter values, which maximize RI
27        prediction_transformed = select_by_labels(features_transformed, labels_predicted)
28        prediction = features_preprocessors.inverse_transform(features_transformed_chosen)
29        return prediction

```

Listing 4.7 Scikit-learn linear model wrapper pseudo-code.

### Multi-Armed Bandit

Originally, the multi-armed bandit (MAB) problem was introduced in [98] and defined as follows: for a given set of choices  $c_i$  with unknown stochastic reward values  $r_i$ , which are distributed normally with variance  $v_i$ , the goal is to maximize the accumulated reward, sequentially selecting several times among available choices  $c_i$ . The problem obtained its name as an analogy to one-hand slot machines in casino and naturally denotes the well-known exploration versus exploitation dilemma.

In most cases, MAB is solved by reinforcement learning (RL) approaches, which analyze the already available evidences before performing each next step. It perfectly fits our requirements of sequential LLH to tackle the problem at hand, therefore, those choices are nothing else, but LLH types (categories of categorical parameter). In [4] the authors proposed the Upper Confidence Bound algorithm as an intuitive MAB solution: in iteration  $k$ , among available categories select one with a maximal UCB value. The UCB for each category is calculated according to Equation (4.1), where first component  $Q$  is a quality of category under evaluation and represents the exploitation portion of UCB. The second component estimates the exploration portion and evaluates the number of times each category was selected. The multiplier  $C$  is a balancing coefficient.

$$UCB = Q + C \cdot \sqrt{\frac{2 \log \sum_1^i n_k^i}{n_k}} \quad (4.1)$$

In this work we implement a proposed in [76] Fitness-Rate-Average-based MAB (FRAMAB) with two

reasons: (1) it is an intuitive and robust approach, (2) according to the benchmarks in [42] it outperforms other MAB algorithms. In FRAMAB,  $n_k^i$  denotes the overall number of categories, while  $n_k$  is a number of times the category under evaluation was selected. The quality estimation  $Q$  in FRAMAB is the average improvement, obtained by the underlying category.

As for the balancing coefficient  $C$ , the authors in [42] were evaluating a range of values between  $10^{-4} \dots 10^{-1}$ . The dominance of  $C$  values for various problem types was different, therefore we expose it to user for configuration.

In addition to the statically defined  $C$  value, we propose a mechanism for  $C$  estimation as a standard deviation in improvement values. The motivation for this is the following: if there exists an uncertainty in category domination, the deviation will be high and it should encourage the exploration portion of UCB values. We do not provide a pseudo-code for this model implementation, since it straightly repeats the algorithm description provided above.

### 4.4 Low Level Heuristics

When our HLH is ready to solve an OP, the time comes to provide the tools for solving. A role of LLH in our hyper-heuristic (HH) may play every algorithm starting from a single heuristic and ending with meta-heuristic (MH) or even other HH. As we discussed in Section 2.2.2, nowadays the MH research is referred to as the framework growth time. Therefore, we are able not only to reuse a single meta-heuristic but to instantiate a set of underlying heuristics among available in relative frameworks. Thus, in this Section we present a review of several meta-heuristic frameworks with an intent to select the best suited one, implement a facade for framework usage and utilize the available algorithms as LLHs in our hyper-heuristic.

Before diving into a description, we briefly outline the LLHs characteristics with respect to which we analyze each framework:

1. **Set of meta-heuristics**, which we will be able to use as LLHs in our HH.
2. **Exposed hyper-parameters**, which are required for LLH tuning. We point it out explicitly, since it happens so that the parameters of an algorithm are exposed not fully.
3. **Set of supported optimization problems**, which will define the applicability of our HH. The wider this set is, the more use-cases developed HH is able to tackle.
4. **Warm-startup**, which is required to continue the problem solving from a previously reached solution. The underlying LLH should not only report the finally found solution(s), but also accept them as the starting points.
5. **Termination criteria**, which are needed to control the intermediate results of optimization process by HH. In our system we use the wall-clock time termination to stop the LLH and report the results.

#### 4.4.1 Low Level Heuristics Code Base Selection

We distinguish the following frameworks as the LLH code basis candidates: Solid<sup>1</sup>, mlrose<sup>2</sup>, pyTSP<sup>3</sup>, LocalSolver<sup>4</sup>, jMetalPy<sup>5</sup> and jMetal<sup>6</sup>.

**Solid.** A framework for gradient-free optimization. It comprises a wide range of MH skeletons with exposed hyper-parameters: genetic algorithm, evolution algorithm, simulated annealing, particle swarm optimization, tabu search, harmony search and stochastic hill climbing. The support of warm-startup is not provided and it requires changes in each algorithm as a consequence of the shared base class absence. Available algorithms do not provide times-based termination criteria and have only evaluation-based and quality-based stop criteria.. Once again, to add a new criterion, one should modify the code of all algorithms. The framework does not provide the problem instances, nor domain-dependent parts of algorithms, therefore, to use it one will need to carry out not only a domain-specific adaptation, but also a problem description.

**mlrose.** A framework with implementation of various well-known stochastic optimization algorithms, such as: naive and randomized hill climbing, simulated annealing, genetic and mutual-information-maximizing input clustering (MIMIC) algorithms. Each listed solver is implemented with an exposed set of hyper-parameters. It is possible to control an initial state, which is handy in our case. As for the implemented OPs, the framework comprises a large set of different types: one max, flip-flop, four and six peaks, continuous peaks, knapsack, traveling salesman, n-queens and max-k color optimization problems. The proposed termination criteria are represented only by one criterion controlling the number of TS evaluations. As in the previous framework, here the algorithms do not share the same code basis, therefore, it may require much effort for their adaptation in general and to introduce a new termination criterion in particular.

**pyTSP.** A system, specially designed to tackle the traveling salesman problem. Together with visualization techniques, it also provides a wide bunch of different algorithms. Here, they are divided into four groups. First group consists of construction heuristics with nearest neighbor, nearest insertion, farthest insertion and cheapest insertion algorithms. Second one is a linear programming algorithm. Third group consists of are perturbation heuristics among which pairwise exchange, also known as 2-opt, node insertion and edge insertion. Fourth group is formed from meta-heuristics and represented by the genetic algorithm. As one may expect, the only supported problem type here is the TSP, moreover, the representation of problem does not follow a broadly used in research community manner. The other drawbacks of this framework are partial hard-coding of hyper-parameters and an absence of exposed termination criteria. Also, the construction heuristics by their nature do not expose the possibility to feed them with the initial solutions. However, in some other algorithms the functionality to specify the initial solution is provided.

**LocalSolver.** A commercial optimization tool with free academic license. It is implemented in C++, and the API is exposed to such programming languages as Python, C++, Java and C#. The software implements a local search programming paradigm [7, 8], therefore, the algorithm itself and its parameters

<sup>1</sup>Solid GitHub repository <https://github.com/100/Solid>

<sup>2</sup>mlrose GitHub repository <https://github.com/gkhayes/mlrose>

<sup>3</sup>pyTSP GitHub repository <https://github.com/afourmy/pyTSP>

<sup>4</sup>LocalSolver website <https://localsolver.com>

<sup>5</sup>jMetalPy GitHub repository <https://github.com/jMetal/jMetalPy>

<sup>6</sup>jMetal GitHub repository <https://github.com/jMetal/jMetal>

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are not exposed. It is required from the user to provide a solver-specific problem description. Thanks to a detailed documentation, the desired TSP example could be found among numbers of other optimization problems. Two possible termination criteria are exposed: a wall-clock time and a number of solver iterations. Also, the framework supports a possibility to set an initial solution for the solver, therefore, it looks like a good candidate for the LLH. Unfortunately, our trial to use the tool showed up that the provided academic license could not be easily used within BRISv2 containerized architecture. A possible work-around is to deploy a license server on a host machine and force workers to register themselves, but we found this to be an expensive task requiring much implementation effort.

**jMetalPy.** An open-source meta-heuristic framework for multi- and single-objective optimizations. Among the provided single-objective algorithms one will find genetic algorithm, evolution strategy, local search (hillclimber) and simulated annealing. Even if the list of proposed heuristics is not the largest in comparison to other reviewed frameworks, every implemented algorithm exposes its hyper-parameters for tuning. We also found the code to be well-structured, therefore, in case of required changes they could be made with less effort. A functionality for heuristic solver warming-up is available out-of-the-box. The various termination criteria are ready as well, among which the wall-clock time-based and the number of TS evaluations-based criteria. The list of supported single-objective optimization problems consists of knapsack, traveling salesman and four other synthetic problems: one max, sphere, Rastrigin and subset sum.

**jMetal.** A meta-heuristic framework implemented in Java is an alternative to previously reviewed Python-based jMetalPy. This framework also provides meta-heuristics for multi- and single-objective OP. For SO OP, jMetal developers implemented the following algorithms: naive and covariance matrix adaptation evolution strategies (CMA-ES), genetic, particle swarm (PSO), differential evolution and coral reef optimization algorithms. It is worth to mention that not all solvers are universally applicable to a wide range of OPs. For instance, CMA-ES, PSO and differential evolution can be applied only to OPs with continuous numeric input such as synthetic mathematical problems. In contrast to implemented in Python jMetalPy, jMetal supports only one termination criterion, based on number of TS evaluations, and does not support algorithm warming-up at all.

To sum up our discussion, we aggregate the described characteristics in Table 4.2, which is similar to Table 4.1, presented during the HLH code basis selection. Once again, the characteristics qualities are scored into three ordinal values: poor, average and good with respect to provided functionality and required effort for adaptation.

**Table 4.2** Meta-heuristic frameworks characteristics.

Characteristic	Solid	mlrose	pyTSP	LocalSolver	jMetalPy	jMetal
Set of heuristics	Poor	Poor	Good	N/A	Average	Good
Exposed hyper-parameters	Good	Good	Poor	Poor	Good	Good
Provided OPs	Poor	Good	Poor	Good	Average	Average
Warm-startup support	Poor	Good	Poor	Good	Good	Average
Termination criteria	Average	Average	Poor	Good	Good	Average

Our ultimate goal is not to reach the best performance in provided solution, but to investigate, whether a proposed concept is able to outperform the baseline performance measures. Thus, while selecting LLH, the quality of provided heuristics and their hyper-parameters are playing a crucial role. For our

experiments we decided to use three LLHs: two MHs from Python-based jMetalPy (simulated annealing and evolution strategy) and one from Java-based jMetal (evolution strategy).

#### 4.4.2 Scope of Low Level Heuristics Adaptation

The selected frameworks propose many algorithm implementations. Since the same people are developing both jMetal and jMetalPy, the overall architecture of both frameworks is similar. Nevertheless, the proposed features are slightly different. For instance, jMetal does not provide time-based termination, nor warming-up the solver by initial solutions. Therefore, we split the adaptation of frameworks onto two parts, one is dedicated to jMetalPy and in the other we discuss jMetal.

**jMetalPy.** During the analysis above, we have found that the provided features greatly fit our requirements. Even if the lists of implemented MHs and supported OPs are not that wide, we could simply reuse the provided out-of-box implementations. In order to do, we implement a framework wrapper (see Listing 4.8), which creates a desired optimization problem instance, MH solver instantiate with the provided hyper-parameters (line 3). Later, we call this wrapper to start a solver execution and report the results in a framework-independent way (line 5). To prevent an expensive problem instances loading within one optimization session, we cache it in memory (lines 8-9). Also, we cache expensive I/O introspection calls, which are used to find framework components: algorithms, termination criteria or different algorithm operators such as mutation, selection, crossover, etc. (lines 11-15).

```

1 class JMetalPyWrapper(ILLHWrapper):
2
3     def construct(hyperparameters: Mapping, scenario: Mapping, warm_startup_info: Mapping) -> None
4         # Constructing meta-heuristics initialization arguments, attach initial solutions
5     def run_and_report() -> Mapping
6
7     # jMetalPy framework introspection helper methods
8     @lru_cache()
9     def _get_problem(problem_name, init_params)
10
11     @lru_cache()
12     def _get_algorithm_class(mh_name)
13
14     @lru_cache()
15     def _get_class_from_module(name, module)

```

**Listing 4.8** jMetalPy framework wrapper pseudo-code.

While experimenting with the framework, we found several implementation flaws in algorithms or their components. The fixes for these bugs were submitted as contributions<sup>12</sup> to implemented open-source framework.

**jMetal.** In contrast to jMetalPy, this framework is implemented in Java, therefore, we cannot perform the software instantiating straightforwardly, since BRISEv2 workers are based on Python. There are several libraries, which allow executing a Java code within Python: JPyype<sup>3</sup>, Py4J<sup>4</sup> or PyJNIus<sup>5</sup>. The usage of one among listed modules enables us to build the same framework wrapper, as we did in previous

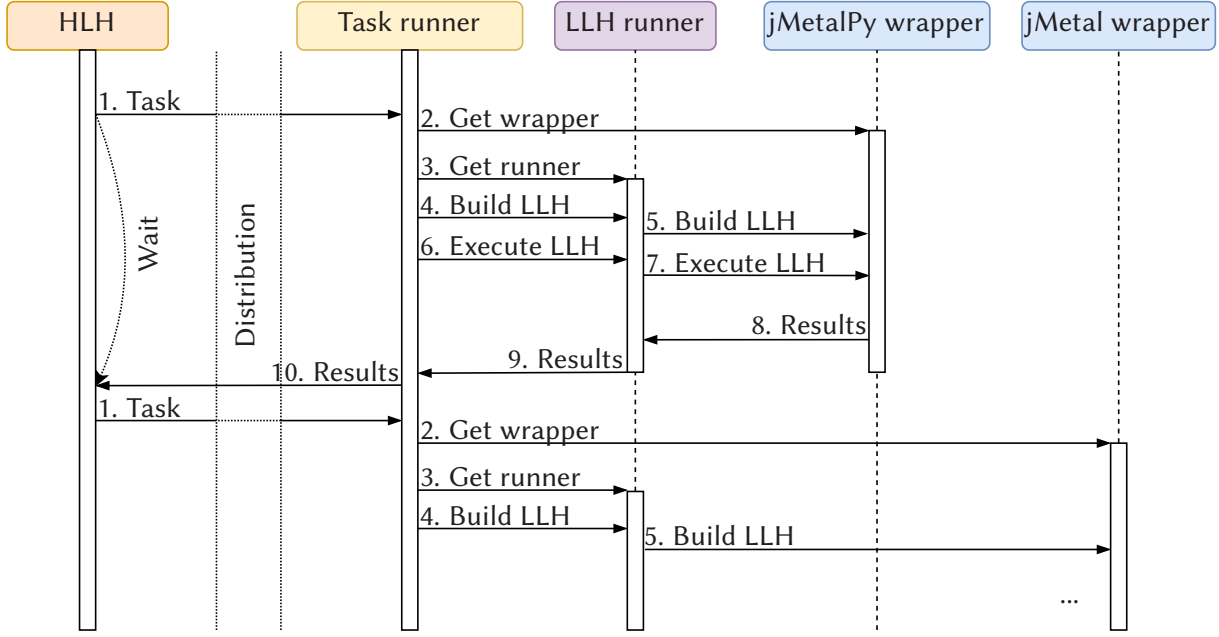
<sup>1</sup>jMetalPy PR 1: <https://github.com/jMetal/jMetalPy/pull/67>

<sup>2</sup>jMetalPy PR 2: <https://github.com/jMetal/jMetalPy/pull/80>

<sup>3</sup>JPyype GitHub repository: <https://github.com/jpyype-project/jpyype/>

<sup>4</sup>Py4J GitHub repository: <https://github.com/bartdag/py4j>

<sup>5</sup>PyJNIus GitHub repository: <https://github.com/kivy/pyjnius>



**Figure 4.1** The low-level heuristic execution process.

case. Since currently we are planning to use only one meta-heuristics, the implementation of such wrapper will be unreasonable. Thus, to use a provided in jMetal evolution strategy, we pack it into an executable file with exposed parameters and call it from worker script, providing hyper-parameters settings and warming-up solutions.

#### 4.4.3 Low Level Heuristic Runner

When the MH wrappers are ready, we use them as different execution strategies of low level heuristic with unified *ILLHWrapper* interface. To operate these wrappers we implement a separate entity: *LLH runner*. It forwards the construction and execution commands to the wrapper, tracks the state, makes general information logging and passes the results after execution back to HLH. This enables us to easily scale workers horizontally, since they are homogeneous and state-less (not taking into account the caching mechanisms). The resulting process of LLH execution from the worker perspective is represented as a sequence diagram in Figure 4.1. Please note, within an implemented approach the meta-heuristics are reinitialized at each external iteration (between each task execution). Therefore, algorithms as simulated annealing are *restarting* between tasks dropping such internal parameters as temperature (in SA) to its initial state.

## 4.5 Conclusion

The performed implementation of proposed in Chapter 3 concept was done by reusing the existing frameworks. The hyper-heuristic is mostly based on the modular BRISv2 framework for parameter tuning. We utilize BRISv2 prediction models in the form of reinforcement learning as a HLH, while several homogeneous workers are carrying out the optimization process using their LLHs. For the LLHs implementation we reuse the existing meta-heuristic frameworks jMetalPy and jMetal. Despite the selected code basis, the proposed approach could be implemented in most of the parameter tuning



systems following SMBO methodology, however, requiring the adaptation according to our review in Section 4.1.

While adapting BRIS<sub>Ev</sub>2, we were forced to set aside the previously used search space representation and implement our own to handle the tiered configuration prediction process and the sparseness issue. An intermediate entity *predictor* was added to decouple the search space shape from the learning-prediction process. It allowed us to extend the previously available models with the several others: fitness-rate-average based multi-armed bandits (FRAMAB) for categorical parameter selection and linear regressors from Scikit-learn framework as surrogates models. We also decoupled data preprocessing steps by reusing the respective tools from Scikit-learn framework.

We believe the proposed implementation will serve well not only as a hyper-heuristic, but also as already well-known and used parameter tuning framework.



## 5 Evaluation

The concepts of search space representation and prediction processes were proposed in Chapter 3. Based on them, in Chapter 4 we implemented a generalized parameter control for meta-heuristics, selection hyper-heuristic and the hyper-heuristic with parameter control approaches. In this Chapter we propose a broad evaluation of the implemented approaches. Experiments may be performed in a number of investigation directions, starting from the developed RL performance comparison to the baseline and ending with the scalability to different problem sizes.

We start this Chapter with a brief presentation of the optimization problem at hand in Section 5.1 and short environment description in Section 5.2. We perform a parameter tuning of low-level heuristics in Section 5.3, which will be used later through our tests for comparison.

The evaluation presented in this thesis could be divided into two main parts:

The first part (Section 5.4) is dedicated to the developed concept analysis in comparison to the baseline. We start the concept evaluation with planning in Section 5.4.1 and proceed firstly reviewing the baseline in Section 5.4.2, secondly the generic parameter control is presented in Section 5.4.3, followed by the selection hyper-heuristic with static hyper-parameters in low-level heuristics review in Section 5.4.4 and ending with the selection hyper-heuristic with parameter control in low-level heuristics review presented in Section 5.4.5.

In the second part (Section 5.5), we investigate an influence of hyper-heuristic with parameter control settings on its performance. In order to do so, once again we firstly perform the experiment planning in Section 5.5.1. Afterwards, in Section 5.5.2 we investigate an influence of a learning granularity on the HH-PC performance. In Section 5.5.3 we check learning models configurations and in Section 5.5.4 we verify the influence of inter-LLH communication configuration.

Finally, Section 5.6 concludes our evaluation with a discussion of the obtained results.

### 5.1 Optimization Problem

In this thesis we are tackling a vehicle routing problem – the traveling salesman OP. We present its short definition here, including the related to benchmark details, however, the detailed explanation could be found in Section 2.1.1: “Given a set of cities and the distances among them, find the shortest path, which visits all cities”. It is a combinatorial OP with a number  $n = N!$  of possible solutions. In our benchmarks we use several instances of symmetric TSP (distances  $x_i \rightarrow x_j$  and  $x_j \rightarrow x_i$  are equal) from a publicly available and broadly used in research TSP benchmark set TSPLIB95<sup>1</sup>. The advantage of choosing this benchmark set lays in a broad compatibility of solvers and frameworks (including jMetal and jMetalPy) with this standardized TSP instance description. The TSP in this case is defined as a set of city coordinates. Therefore, before starting to solve a problem, the distance matrix is usually built by heuristic, calculating the Euclidean distances between each pair of cities. For a more detailed explanation of the problem instance description proposed in TSPLIB95, please refer to [95].

For our benchmarks we select four problem instances: *kroA100*, *pr439*, *rat783* and *pla7397* of sizes 100, 439, 783 and 7397 cities respectively. The optimal tours for each of these problem instances were

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<sup>1</sup>TSPLIB95 website: <http://comopt.ifl.uni-heidelberg.de/software/TSPLIB95/>

previously obtained by the exact solvers and reported in aforementioned library. We present the optimal solutions in Table 5.1.

**Table 5.1** TSP instances optimal tour length.

TSP instance	Optimal tour length
kroA100	21282
pr439	107217
rat783	8806
pla7397	23260728

## 5.2 Environment Setup

We run our experiments with an enhanced by our approach BRISv2 and deploy it in Docker containers on host machine with the following characteristics:

- **Hardware:** Fujitsu ESPRIMO P958 computer with 64GB 2667MHz RAM (16GB \* 4 pcs), Intel Core i7-8700 CPU @ 3.2 GHz (6 cores \* 2 threads) and Samsung 1TB SSD.
- **Software:** GNU/Linux Fedora 29 host OS and installed Docker engine version 1.13.1.

We deploy 6 homogeneous BRISv2 workers with LLHs on the same host machine and run each experiment 9 times to gather the statistics. Each execution was performed with wall-clock-based termination criterion configured to shut down the optimization session after 15 minutes.

## 5.3 Meta-heuristics Tuning

As we conclude in Section 2.3.4, the goal of parameter control is at least to reach the parameter tuning approaches results quality. Therefore, before running the major set of evaluation experiments, we have to perform a parameter tuning for the underlying LLHs.

### 5.3.1 Parameter Tuning System Configuration.

As a tuning system, we use our concept implementation in the tuner mode. As mentioned in Section 3.5, to enable the parameter tuning mode we built a search space based on a single LLH with its parameters and disable the solution transfer between configurations. In our particular case we define three search spaces for each underlying meta-heuristic. We run the tuning for 8 hours on 10 deployed worker nodes and give three minutes for each task (configuration) evaluation. The underlying prediction mechanism was configured to use TPE with 100% window size. We disable the repetition strategy and outliers detection leaving each configuration evaluated only once, since our preliminary experiments showed that the variance among evaluations is negligible.

### 5.3.2 Target Optimization Problem and Search Space of Parameters.

The role of optimization problem at hand is played by one of the selected TSP instances: *rat783*. We base the algorithms tuning on this instance, since it is a middle-size problem among the instances selected for evaluation.

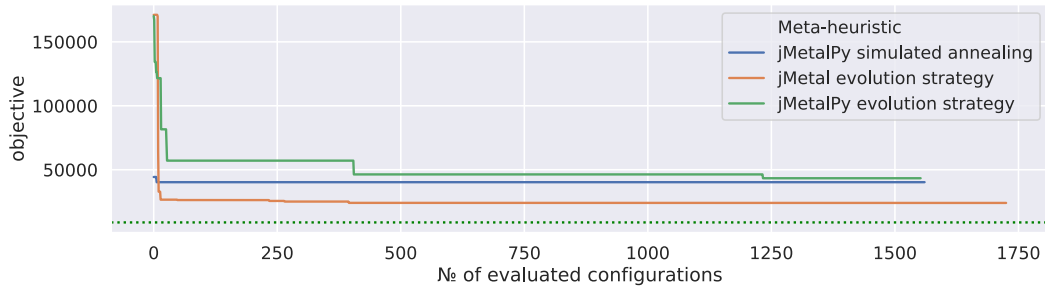
**jMetalPy evolution strategy.** This meta-heuristic is implemented as a naive evolution strategy, however, we found an important recombination mechanism missing, therefore, the heuristic is acting mostly by means of mutation operations. As a configuration, it requires several hyper-parameters of different types. Integer parameter  $\mu$  (*mu*), which denotes a number of parents in the population. Integer parameter  $\lambda$  (*lambda*) defines a number of offspring. We tune both parameters in range  $[1..1000]$ . Boolean parameter *elitist* defines a selection strategy, where *true* value enables elitist selection ( $\mu + \lambda$ ), while *false* value disables it ( $\mu, \lambda$ ) (more details in Section 2.2.2). Also, the framework proposes two possible *mutation types* for combinatorial OPs: *permutation swap* and *scramble mutation*. The mutation probability is tuned in range  $[0..1]$  respectively.

**jMetalPy simulated annealing.** In this meta-heuristic authors defined the solution neighborhood by means of the same aforementioned mutation operators. Thus, we use them and similar mutation probability range for tuning the SA. Unfortunately, the authors did not provide other, but exponential cooling schedule and did not expose *temperature* or *alpha* (cooling rate) parameters. This is the reason for a such tiny parameter space for this MH.

**jMetal evolution strategy.** In this meta-heuristic a set of exposed hyper-parameters is almost the same, as for previously described Python-based evolution strategy implementation. The only difference is that the mutation type is fixed, therefore, we exclude it from the parameter space, but leaving the mutation probability and elitist parameters. All the other parameter ranges are the same as for the defined above ES.

### 5.3.3 Parameter Tuning Results.

The process of parameter tuning is depicted in Figure 5.1. 8 hours of tuning on 10 workers with 3 minutes for each configuration resulted in at least 1500 evaluated parameter combinations.



**Figure 5.1** The low level heuristics parameter tuning process on rat783 TSP instance.

In the figures below, we propose a visual analysis of the results. We separately present the numerical and categorical parameters for each meta-heuristic.

The numeric hyper-parameters are presented as scattered points of parameter value (*x-axis*) and the respective objective function result (*y-axis*), obtained for configuration with this parameter value. Although, such an isolated approach to analyze data may be error-prone. But still, it is enough to get a birds-eye view on the existing dependencies. To represent trends among the numeric parameter values we draw the regression line (4<sup>th</sup> degree) in green. At the top and to the right side of the plot value densities are presented. From the top density one can derive, which parameter values were sampled more often, while densities on the right side show, which objective values and how often were obtained.

As for the categorical parameters, we plot their values in violin plots. It is a combination of box plot and kernel density plot. Since all categorical parameters of underlying algorithms have only two values, each side of violin plot shows, which objective results and how often was obtained for the respective category. We also distinguish values by different colors, while the violin shape shows an expected probability of the respective result value. Inside the figure we also draw three dashed lines. A middle line with long dashes is a median, while lower and upper lines with short dashes show first and third distribution quartiles respectively.

**jMetalPy evolution strategy parameters.** In Figure 5.2 one may clearly see an explicit dependency between the number of parents (parameter *mu*) and the objective function: by setting lower number of parents, better results are obtained more often. However, the offspring number dependency is not that clear (parameter *lambda*). We may see that a high offspring number does not tend to provide good results, but the number of performed estimations for low *lambda* is not enough to be strongly ensured that this value is better. Yet, even with a small number of observations we may guess that a low *lambda* is a good parameter value choice. With respect to the mutation probability, it may be observed that higher rates tend to produce better results.

As for the categorical parameters presented in Figure 5.3, one may see a strong bias towards good results appears when using elitist algorithm version. Concerning the mutation type, the dominance is not obvious, but permutation mutation slightly outperforms scramble type.

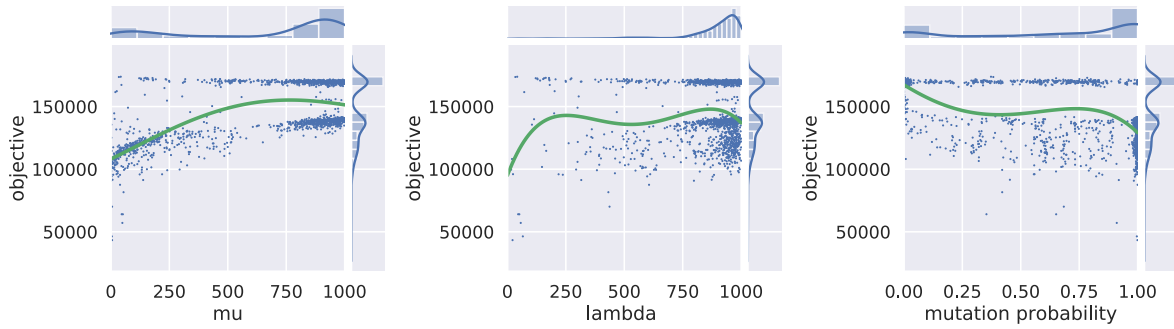


Figure 5.2 jMetalPy evolution strategy numeric hyper-parameters tuning.

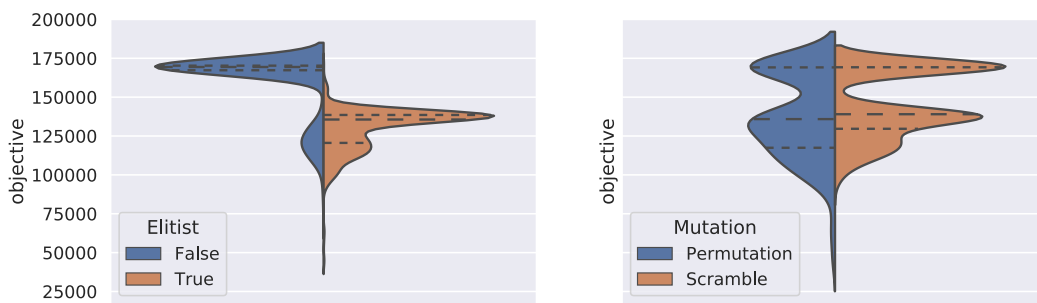
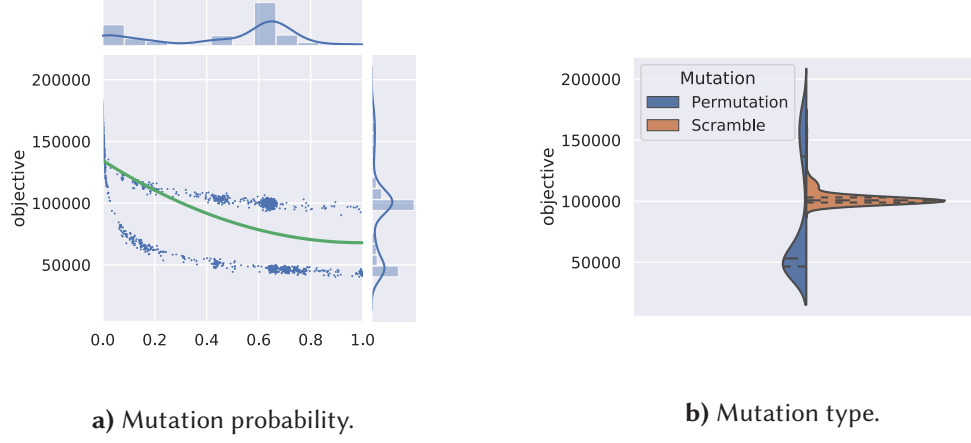


Figure 5.3 jMetalPy evolution strategy categorical parameters tuning.

**jMetalPy simulated annealing parameters.** In this meta-heuristic only two parameters were tuned: categorical mutation type, the results of which are presented in Figure 5.4b and numerical mutation probability depicted in Figure 5.4a. One may see a strong dominance of permutation mutation type, while scramble produces average, but rather stable results. The mutation probability trends are also clear:

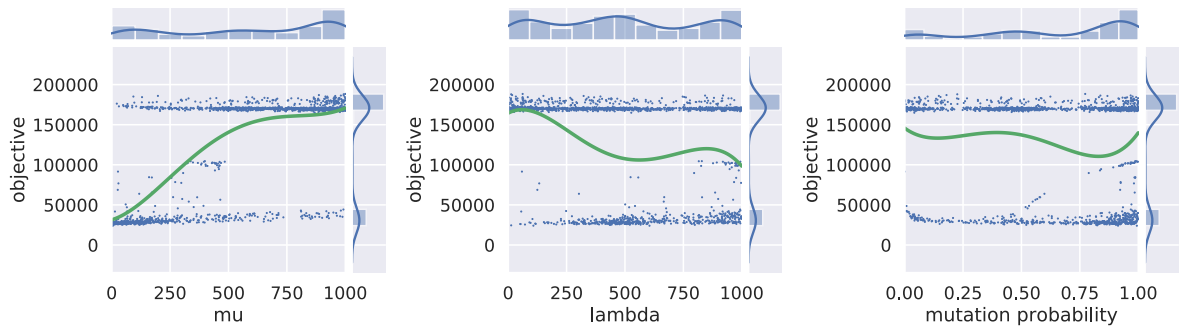


higher parameter values produce better results. Indeed, the dependency on the mutation probability is obvious, since the underlying algorithm is performing the search space traversal by means of solution mutation. The two clear lines of results, which can be viewed in Figure 5.4a are correlated with the mutation types: lower corresponds to permutation mutation type usage, while upper is the result of scramble mutation usage.



**Figure 5.4** jMetalPy simulated annealing parameters tuning.

**jMetal evolution strategy parameters.** The final heuristic under investigation is a Java-based implementation of evolution strategy. At the first glance, the regression lines are not looking the same as for jMetalPy.ES, but the overall trends are similar: lower values of  $\mu$  parameter result in better objective, while the mutation probability should be high. In contrast to jMetalPy.ES, here the middle-range values of  $\lambda$  parameter tend to produce the best results. The difference may be explained by the performance degradation of Python-based algorithm with large offspring number: the required computational effort for accomplishing the iteration increases, while Java-based version could handle a larger number of offspring. A dominance of elitist algorithm version is not obvious, but comparing the first quartiles positions, one will agree that elitist ES version is better.



**Figure 5.5** jMetal evolution strategy numeric parameters tuning.

We collect the best performing configurations of each meta-heuristic in Table 5.2. We also highlight here the default values for each parameter, which were selected with the motivation of being in the values ranges middle.

**Table 5.2** Static hyper-parameters of low-level meta-heuristics.

Hyper-parameter	Default value	Tuned value	Parameter values range
<i>jMetalPy evolution strategy</i>			
$\mu$	500	5	[1..1000]
$\lambda$	500	22	[1..1000]
elitist	False	True	{True, False}
mutation type	Permutation	Permutation	{Permutation, Scramble}
mutation probability	0.5	0.99	[0..1]
<i>jMetalPy simulated annealing</i>			
mutation type	Permutation	Permutation	{Permutation, Scramble}
mutation probability	0.5	0.89	[0..1]
<i>jMetal evolution strategy</i>			
$\mu$	500	5	[1..1000]
$\lambda$	500	605	[1..1000]
elitist	False	True	{True, False}
mutation probability	0.5	0.99	[0..1]

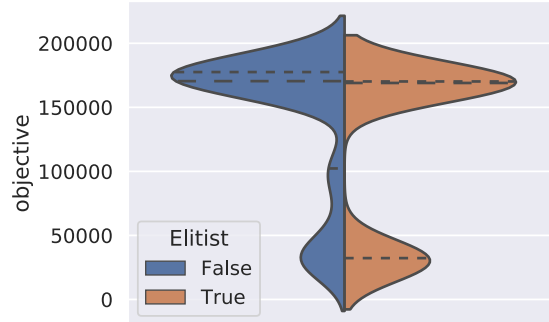
## 5.4 Concept Evaluation

### 5.4.1 Evaluation Plan

To evaluate the developed approach performance, at first we need to define the baseline. In most cases it is an isolated meta-heuristics, which are solving the OP using static hyper-parameters. However, to evaluate the applied generic parameter control to meta-heuristic, we must take a closer look on the respective meta-heuristic results with tuned in offline and controlled in online hyper-parameters. For the selection hyper-heuristic analysis, we compare the performances of all underlying MHs running separately and united together within our hyper-heuristic. Please note, in this case the hyper-parameters are static. To evaluate the selection hyper-heuristic with parameter control in low-level heuristics, we compare it to separately running underlying meta-heuristics with tuned parameters. In order to organize the evaluation plan, we distinguish two stages of configuration construction. At the first stage, the LLH selection occurs, while at the second stage, our system selects the respective hyper-parameters. At either stage we may use different prediction approaches.

To select the LLH, apart from random and static selection we also use FRAMAB and Bayesian ridge regression model (BRR) from Scikit-learn framework (see Section 4.3.3). Please note, for the Bayesian ridge regression we use default parameters, which could be found in the framework documentation<sup>1</sup>. The accuracy threshold for BRR construction equals to 0.5 (see details in Section 4.3.3). We set a single FRAMAB parameter  $C$  to be equal to  $STD$  (see details in Section 4.3.3).

To select the LLHs hyper-parameters, apart from static default and tuned values we also use random

**Figure 5.6** jMetal ES elitist parameter tuning.

<sup>1</sup><https://scikit-learn.org>

selection, a previously available in BRISEv2 TPE with default values (split size equals to 30%) and the mentioned above BRR. To perform a random search-based surrogate optimization, we sample 96 (default BRISEv2 configuration) parameter values combinations for each search space level.

The set of used sampling techniques is presented in Table 5.3.

**Table 5.3** Sampling techniques used for the concept evaluation.

LLH selection	LLH parameters selection
1. Random	1. Default
2. Multi-armed bandit	2. Tuned beforehand
3. Bayesian ridge regression	3. Random
4.1. Static jMetalPy.ES	4. Tree Parzen Estimator (TPE)
4.2. Static jMetalPy.SA	5. Bayesian ridge regression (BRR)
4.3. Static jMetal.ES	

With this table we pick a set of sampling techniques to form a desired system configuration, which leads to different operation modes. For instance, baseline mentioned above could be formed by code 4.1.1 for jMetalPy evolution strategy, used with the default hyper-parameters, or by code 4.3.2 for jMetal evolution strategy, used with the hyper-parameters tuned in offline.

Our benchmark plan for the concept evaluation looks like a set of following experiment groups:

- **Baseline (MH).** We evaluate each meta-heuristic separately with the default and tuned hyper-parameters: 4.1.1 and 4.1.2 for jMetalPy evolution strategy; 4.2.1 and 4.2.2 for jMetalPy simulated annealing; 4.3.1 and 4.3.2 for jMetal evolution strategy respectively.
- **Meta-heuristics with parameter control (MH-PC).** This set of experiments is dedicated to verify an impact of the generic parameter control on meta-heuristics' performance and includes experiments: 4.1.3, 4.2.3, 4.3.3 to investigate the influence of random parameter allocation; 4.1.4, 4.2.4, 4.3.4 to verify TPE-based parameter control and 4.1.5, 4.2.5, 4.3.5 to probe BRR-based parameter control.
- **Selection hyper-heuristic with static parameters in LLH (HH-SP).** These benchmarks are dedicated to the implemented online selection HH performance investigation. It implies the LLHs usage with static parameters, therefore, we evaluate HH-SP performance with the default and tuned beforehand LLH parameters. The experiment codes are following: 2.1, 2.2 for FRAMAB-based HH-SP and 3.1, 3.2 for BRR-based HH-SP with default and tuned parameters respectively.
- **Selection hyper-heuristic with parameter control in LLH (HH-PC).** It is a final set of benchmarks for concept evaluation. Here we evaluate an influence of simultaneous online LLH selection and parameter control on optimization results. The benchmark set is encoded with the following experiments: 1.3, 2.4, 2.5, 3.4, 3.5.

The aggregated concept benchmark plan is presented in Table 5.4. The required running time approximately equals to 9 days and 18 hours on a single machine. Please note, the environment setup is presented in Section 5.2.

#### 5.4.2 Baseline Evaluation

As we discussed previously, the comparison of obtained results should be performed with the defined baseline. In this section we review the meta-heuristics performance out-of-the-box on different problem

**Table 5.4** Concept benchmark plan.

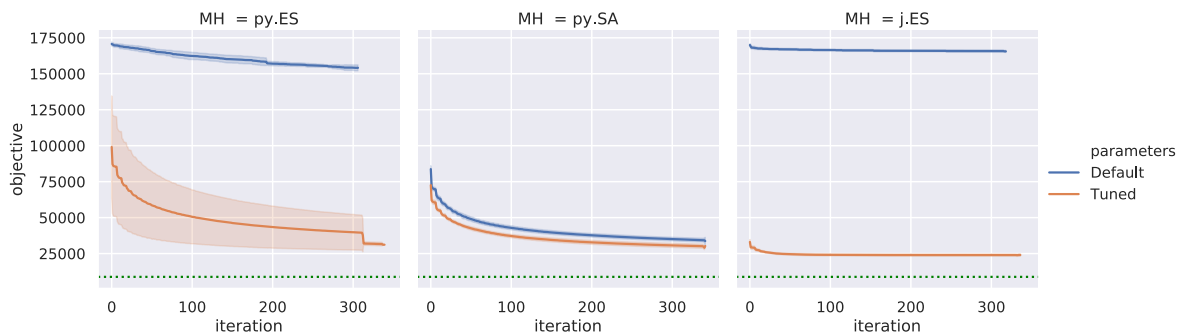
Experiment group	Related codes
MH	4.1.1., 4.2.1, 4.3.1
	4.1.2, 4.2.2, 4.3.2
MH-PC	4.1.3, 4.2.3, 4.3.3
	4.1.4, 4.2.4, 4.3.4
	4.1.5, 4.2.5, 4.3.5
HH-SP	1.1, 1.2
	2.1, 2.2
	3.1, 3.2
HH-PC	1.3
	2.4, 2.5
	3.4, 3.5

sizes and parameter settings. For the visibility reasons, here and on we plot the intermediate and final performance evidence for each problem instance separately. All underlying TSP instances were previously solved by other exact solvers, therefore, we also present an optimal solution, available for each instance as a green dotted line, however, if it appears in a range of interest.

**kroA100 and pr439 TSP instances.** Both 100 and 439 cities TSPs are relatively small problem instances. Therefore, all underlying MHs reach a local optimum after a few first external iterations. A difference between the external and internal iterations is the following: the first ends, when the main node sends the selected configuration and receives its results from the worked node. On the contrary, an internal iteration occurs inside LLH itself. Therefore, since the MHs quickly reach a local optimum on these TSP instances, there is no reason to spend much time on their results review. We put a visual representation of benchmarks for kroA100 and pr439 into the thesis appendix (Appendix A.1.1).

The only observation that is worth mentioning is SA result with tuned parameters. They are worse in contrast to default values on kroA100 TSP instance. It is explained by the fact that for algorithm tuning we used a different problem instance (rat783). It only confirms a motivation of the parameter control approaches: tuning is a problem-dependent technique.

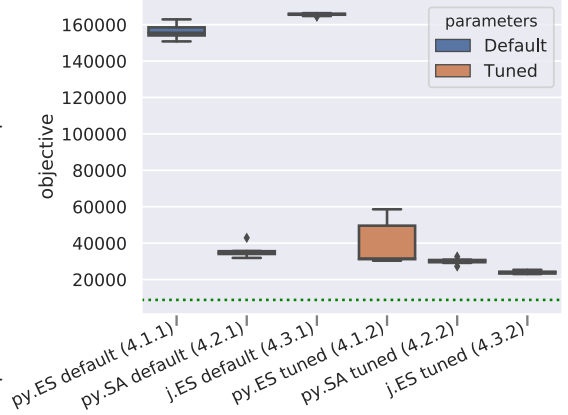
**rat783 TSP instance.** This is an average size problem reviewed in the thesis. The bold lines in Figure 5.7 is a statistical mean for all 9 experiment runs with default (blue line) and tuned parameter values (orange line). A shadow around these lines is a confidence interval derived from 9 repeated runs.

**Figure 5.7** Intermediate results of meta-heuristics with static parameters on rat783.

One may observe how parameter setting differently affects MHs: in evolution strategies the changes in performance is dramatic, while the results of simulated annealing (py.SA) are almost not affected. We also observe a decreased performance stability of tuned jMetalPy ES meta-heuristic (py.ES). It is reflected in a large confidence interval not only of the intermediate results, but also in a final solution quality statistics (Section 5.4.2).

jMetal.ES (j.ES) with default parameters performs extremely slowly. However, using an optimized hyper-parameters it quickly reaches a local optimum (after 50 external iterations) with the best produced results among other heuristics (Figure 5.7 and Section 5.4.2). Analyzing the performance evidence of Python-based solvers, we may conclude that they almost reached local optima in given 15 minutes using tuned parameters, and their final results are slightly worse than the ones produced by j.ES (Section 5.4.2).

**Please note**, the trends' perturbation at the end of presented tuned py.ES is caused by the difference in number of external iterations among all runs (left figure in Figure 5.7, tuned parameters). This number varies, since we used the wall-clock BRISv2 termination criterion, but in some cases due to our implementation flaws LLHs reported with the delay or too hastily, ignoring given 15 seconds running time. Thus, the system managed to perform different numbers of external iterations. The used in this thesis visualization software<sup>1</sup> estimates results average and deviation at each external iteration over all 9 performed runs. Thus, if one (or several) experiment execution(s) managed to perform more iterations than the majority of others, trends on this exceeding iterations will be respectively changed. Unfortunately, this perturbation appears in most of the progress charts, therefore, we perform the comparison of the final results by means of separately presented box-plots.



**Figure 5.8** Final results of meta-heuristics with static parameters on rat783.

**pla7397 TSP instance.** The largest TSP instance investigated in this thesis for a 7.4 thousand of cities is, however, referred to as a middle-size OP in used TSPLIB95. With this instance, the performance evidence were changed the most, therefore, we discuss each MH behavior separately.

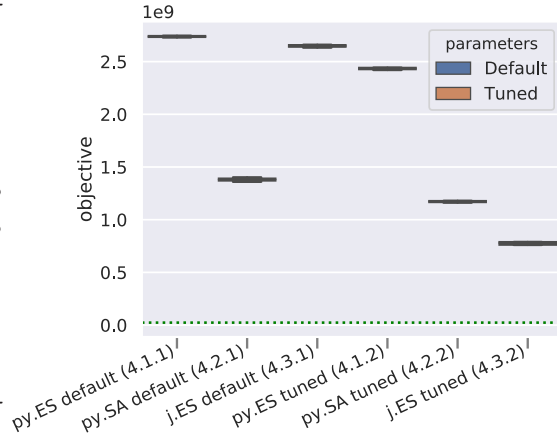
Python-based version of ES provides the worst results with both default and tuned parameters. Please note, the number of performed iterations by this MH with default parameters is less 50. It is caused by several reasons. Firstly, the amount of time required to perform an internal LLH iteration increased dramatically. Thus, with specified 15 seconds for one task run, it actually takes much more time (up to 1 minute). It may be caused by the algorithm code basis implementation. To implement generic termination criteria (and some other features) the authors utilized a push-observer design pattern [6], according to which the underlying algorithm triggers its observers after finishing internal iteration. Therefore, the stopping criteria are evaluated only after finishing the iteration, which in case of running py.ES with TSP instance for 7.4 thousand cities takes a while depending on the algorithm configuration. For instance, with parameters  $\{\mu=5, \lambda=10\}$  termination happens in time, while setting  $\{\mu=500, \lambda=500\}$  the required number of computations is much higher, therefore, we observe the ES algorithm termination after a very first internal iteration. This also causes a poor solution quality improvements. Naturally, there is also overhead in the results sending through the network, but

<sup>1</sup>Python Seaborn data visualization framework web page: [seaborn.pydata.org](https://seaborn.pydata.org)

comparing the performance of Java-based ES with default parameter values, this overhead caused the decrease only in 50 external iterations. We also eliminate a possible issue in a required time for problem loading (building the TSP distance matrix), since using problem instance caching (see Section 4.4.2), the worker node does it only once. In any case, this issue requires a deeper investigation that we postpone to the future work due to the time limits. With tuned parameters for py.ES, the issue with task reporting delays disappears and, therefore, the number of external iterations is higher, but the solution improvements are still weak (see left picture on the Figure 5.9).

As in the previous case, py.SA produces good results quality improvements at each external iteration, least depending on the hyper-parameter values. Even with a default configuration, py.SA outperforms the final results of py.ES after the first 50 external iterations. Setting the tuned parameter values, the performance of the algorithm increases, but not dramatically. A resulting progress curve, presented in the middle of Figure 5.9, shows that py.SA requires more time to converge that it was provided and still far from its potential local optima on pla7397 after 15 minutes.

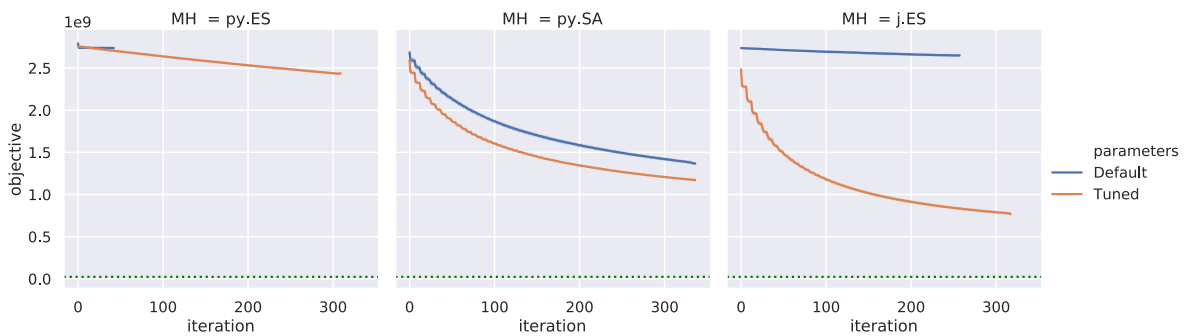
j.ES is a perfect candidate to show, how important is a parameter setting. With default configuration j.ES is weak in making improving steps and cannot compete with other algorithms. Our guess here is the same as for the Python-based version: the number of internal iterations is extremely low for making a good search space traversal. However, a tuned version of j.ES outperforms all other solvers in intermediate (Figure 5.9) and final performance terms (Section 5.4.2).



**Figure 5.10** Final results of meta-heuristics with static parameters on pla7397.

**Discussion.** The observed results of meta-heuristics execution confirmed the algorithm parameter setting problem importance, discussed in Section 2.3. An effect of proper parameter selection is different among available algorithms. In our case, the performance of two out of three solvers is highly dependent on the hyper-parameter settings (ESs). Thus, an application of the proposed in Chapter 3 generic parameter control approach to these algorithms is rather intriguing and may reveal the proposed methodology benefits.

From the other side, we observe the domination of only one algorithm among the others with static parameters. See how all MHs were solving each TSP instance with default parameters: in each case



**Figure 5.9** Intermediate results of meta-heuristics with static parameters on pla7397.



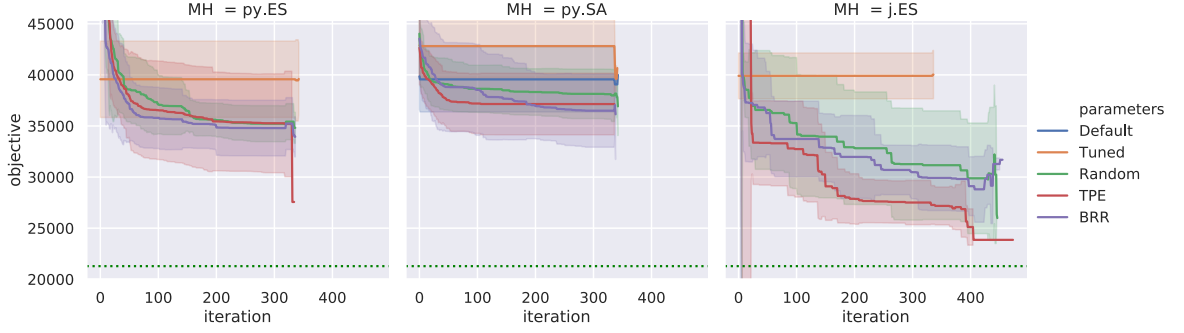


Figure 5.11 Intermediate results of MH-PC on kroA100.

SA outperforms two other ESs. The usage of all three MHs in a selection hyper-heuristic with static hyper-parameters will reveal its applicability. On the contrary, when we switch to the tuned parameter usage, j.ES is preferred. We see it clearly when the MHs are applied to the largest TSP instance and, therefore, we expect to observe this MH dominance in a selection hyper-heuristic with tuned LLHs.

#### 5.4.3 Generic Parameter Control (MH-PC)

As discussed in Section 2.3.3, the goal of dynamic parameter setting is a maximization of underlying algorithm performance measurements at runtime. In this part of evaluation we compare the performance of algorithms with statically defined hyper-parameters (default and tuned) to performance of the same algorithms with enabled generic RL-based parameter control.

**kroA100 TSP instance.** Generic parameter control on a small problem instance is able to outperform the results of static parameters after first 50 iterations on all MHs (Figure 5.11). We may observe that even the random changes hyper-parameters at runtime result in better solutions, comparing with statically defined parameters (Figure 5.12). It is mainly caused by the changes in a neighborhood definition (mutation type) and traversal process (mutation probability). In most cases, given enough time the learning-based parameter assignment outperforms random allocation.

Please note, the number of performed by j.ES iterations in Figure 5.11. According to our plan, time for optimization session equals 15 minutes. We define 15 seconds for running one configuration (external iteration). We run 6 workers in parallel, which in the most optimistic case should perform  $\frac{15 \cdot 60 \cdot 6}{15} = 360$  external iterations. However, we observe even more than 400. After an investigation, we have come to the conclusion that it is caused by an implementation flaw of j.ES. While adding time-based termination

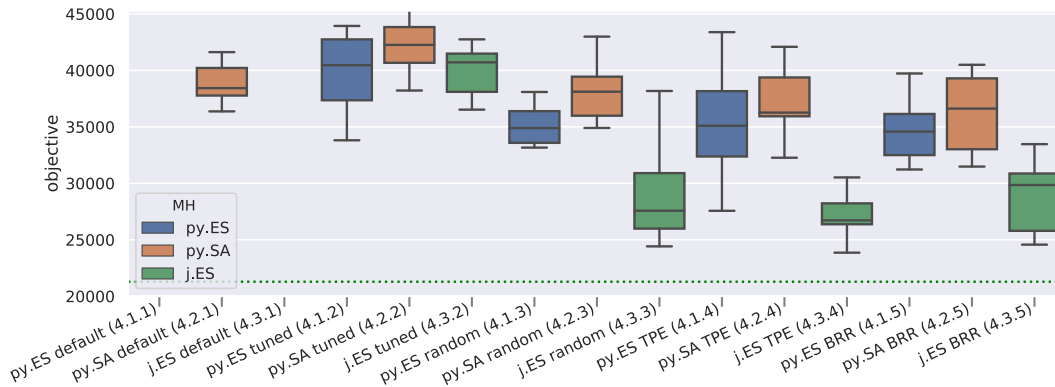
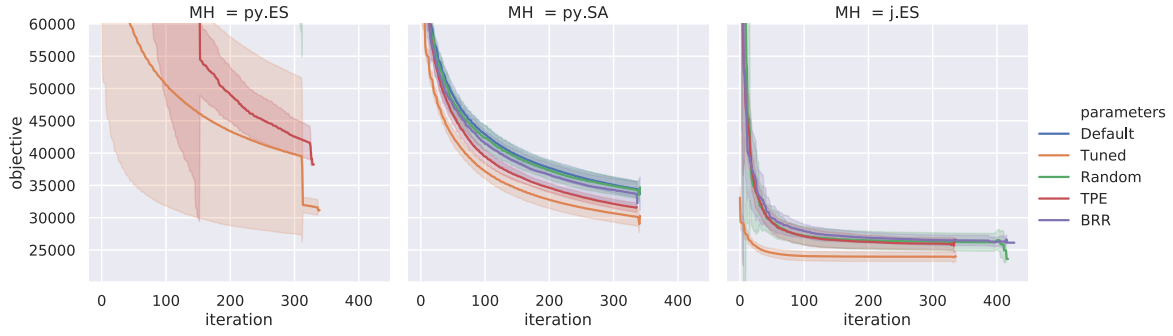


Figure 5.12 Final results of MH-PC on kroA100.

## 5 Evaluation



**Figure 5.13** Intermediate results of MH-PC on rat783.

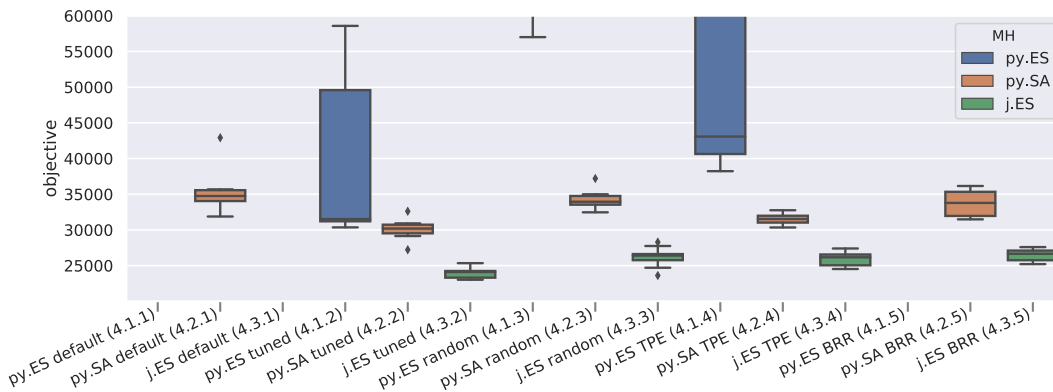
criterion, we did not remove the previously existing iteration-based. For the iteration counter in jMetal meta-heuristics a regular Java integer is used, which we set to its maximal value when using a time-based criterion. Given a ‘light’ algorithm configuration (low  $\mu$ ,  $\lambda$  and mutation probability) and a relatively small OP, MH is able to reach the maximal number of iteration in less than 15 seconds, therefore, terminating earlier and triggering a new external iteration. Certainly, it is our implementation flaw, which should be fixed in a future work.

**pr439 and rat783 TSP instances.** In these two cases, the behavior of solvers was similar, therefore, we decided to join their discussion and present only the plots for a larger instance (rat783). Still, the intermediate and final performance representation for pr439 TSP instance can be found in Appendix A.1.2.

When the parameter control is applied to a larger problem instance, it starts to require more evidence (external iterations) for finding good-performing settings for py.ES. Concretely, the TPE-based parameter control was the closest in approaching the quality of tuned parameters. All techniques produced highly unstable intermediate and final results: please, draw your attention to the left side of Figure 5.13, and filled with blue boxes in Figure 5.14 respectively.

The results of parameter control application to less sensitive py.SA are the following: randomized parameter sampling settled on the level of default parameters quality. BRR-based parameter control yielded a slightly better results, while TPE model approached the quality of tuned parameters (Figure 5.14).

On the contrary, generic parameter control in j.ES MH leads to results quality comparable with tuned parameters (Figure 5.14). Please note, as for previous problem instance, even a random-based parameter sampling outperforms default parameters when given enough time.



**Figure 5.14** Final results of MH-PC on rat783.

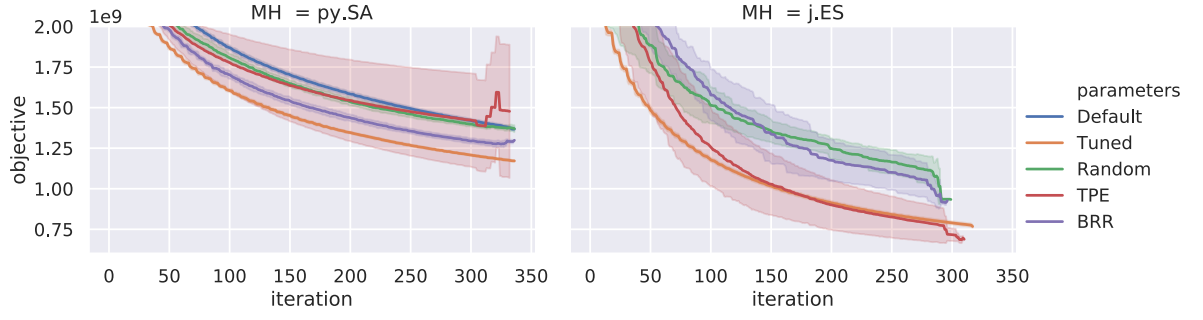


Figure 5.15 Intermediate results of MH-PC on pla7397.

**pla7397 TSP instance.** For the final problem instance we omit the results for py.ES, because it did not manage to perform even the slightest improvement, compared with the default parameter values. It is caused by the fact that in early stages our approach acts as a random search, since not enough evidence were obtained to build prediction models.

As in previous cases, the least configuration-sensitive py.SA shows an ability to perform almost equally with any parameter settings (Figure 5.15). Neither among used control techniques was able to outperform the results obtained by the tuned in offline algorithm (Figure 5.16).

As for j.ES, the model-based MH-PC outperforms the randomized parameter values allocation. Moreover, TPE-based control reached and outperformed even the results of hyper-parameters tuned in offline.

**Discussion.** In general, the review of meta-heuristic performance on different problem instances showed that the proposed generic parameter control approach is able to yield not only the near-tuned parameters quality, but in some cases even outperforming results.

Taking into account the results with random parameter allocation we make two conclusions. Firstly, even randomized parameters changes are able to improve a potentially bad static hyper-parameter setting (j.ES case). Secondly, the learning mechanisms should and must be improved further by means of different surrogate models usage. The proper technique for surrogate optimization should be used. Leaving the improvement steps for future work, we conclude that the developed in this thesis generic parameter control concept may be proposed as a replacement of the parameter tuning for meta-heuristics.

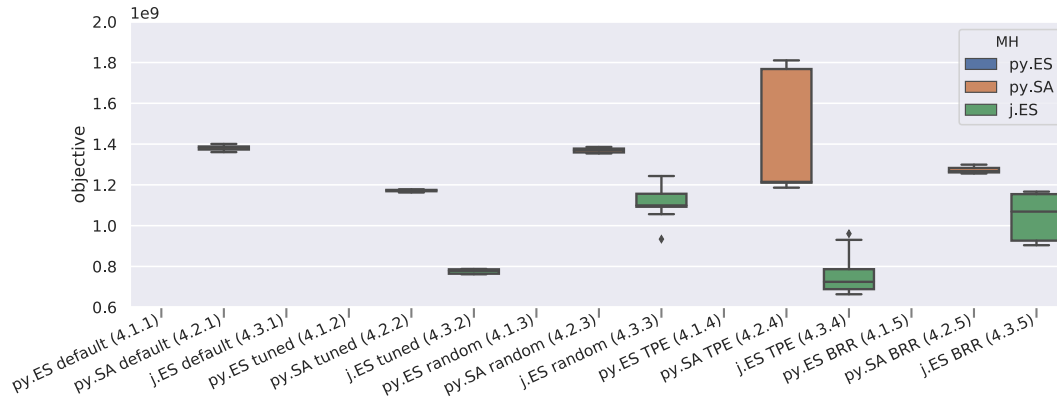
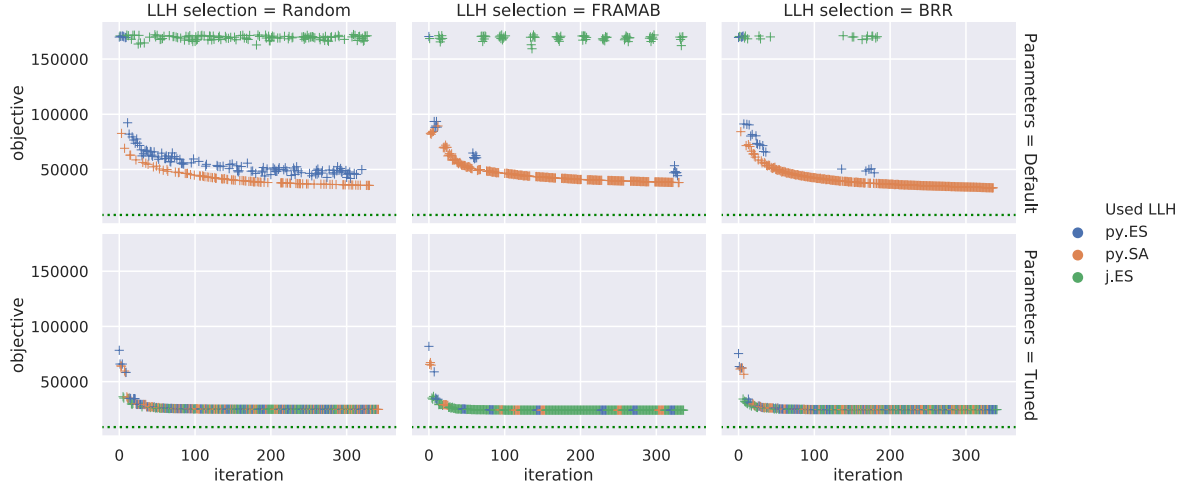


Figure 5.16 Final results of MH-PC on pla7397.

## 5 Evaluation



**Figure 5.17** Intermediate performance of HH-SP on rat783 (single experiment).

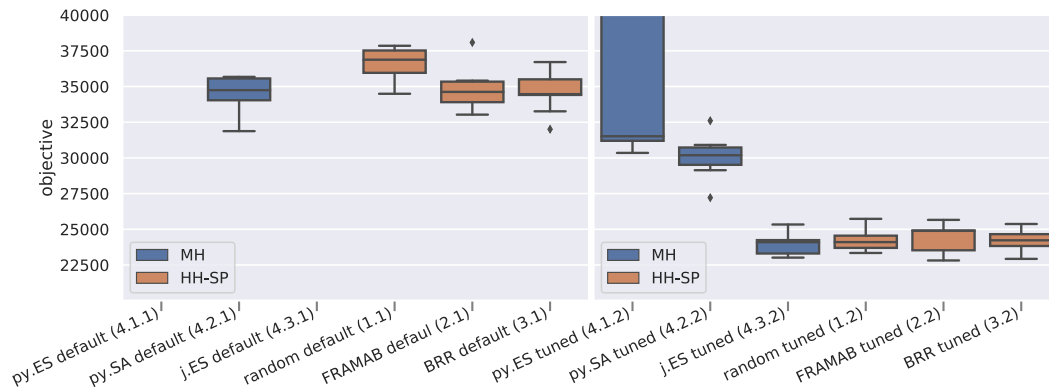
### 5.4.4 Selection Hyper-Heuristic with Static LLH Parameters (HH-SP)

The second mode of the developed approach is the RL-based selection hyper-heuristic, which description can be found in Section 3.5. Here we group three available LLHs (aforementioned py.ES, py.SA and j.ES) with static parameter (default and tuned) into selection hyper-heuristic (HH-SP).

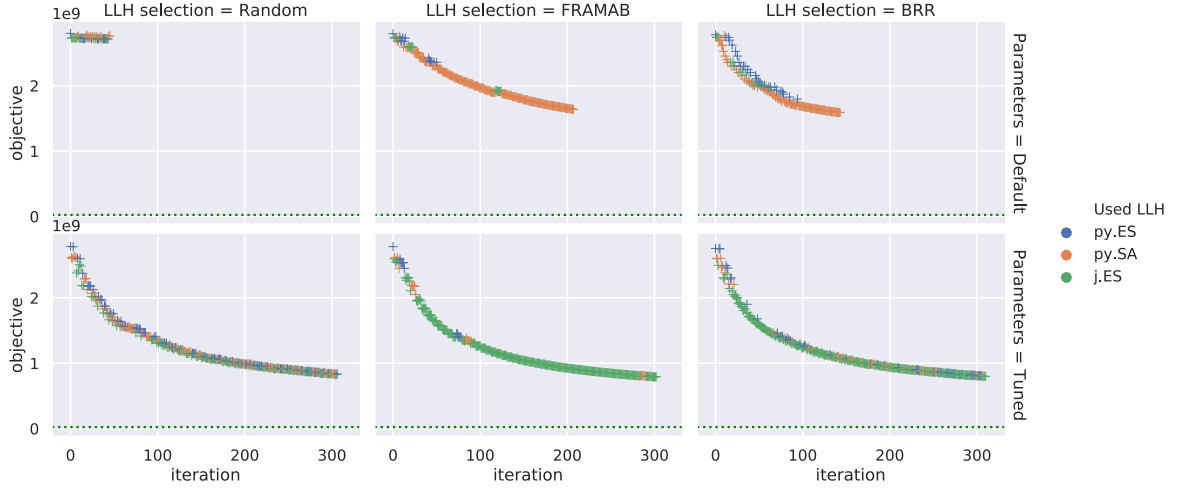
We present the problem-solving process in two forms. Firstly, we distinguish the selected at each external iteration LLH. In order to do so, we visualize only the first repetition (out of 9 available). Secondly, we present the final results of all runs in the form of box-plots and compare them with the performance of underlying LLHs used executed separately (baseline). The left group of box-plots presents the final solution quality obtained with the default parameter values, while on the right site the results of tuned parameters are outlined.

**kroA100, pr439 and rat783 TSP instances.** Once again, we group relatively small problem instances on which the implemented HH-SP performs similarly. To analyze this group, we selected the largest instance among them: rat783, while the figures depicting kroA100 and pr439 TSP instances may be found in Appendix A.1.3.

We would like to draw the readers' attention to HH-SP cases, in which the LLHs were used with the default parameter values (upper row in Figure 5.17). According to baseline evaluation, there is only one algorithm with a strong performance dominance: py.SA. Therefore, in Figure 5.17 we observe a



**Figure 5.18** Final results of HH-SP on rat783 (statistic of 9 runs).



**Figure 5.19** Intermediate performance of HH-SP on pla7397 (single experiment).

high frequency of py.SA sampling by both learning-based selection strategies. One may distinguish a repetitive pattern in LLH allocation with FRAMAB (middle column). It is caused by a deterministic essence of the algorithm. Reaching a critical point, where other heuristics should be verified, the FRAMABs' exploration mechanism fully guides a selection. Due to the time-based LLH termination usage, all workers are starting the next round (mostly) in bunches. Thus, when a new round starts, FRAMAB operates on static information and allocates all next configurations with the same LLH, which turns to be the second best performing algorithm: j.ES. Therefore, we conclude that FRAMAB behaves slightly inertly in our setup. One may argue this will cause a decrease in performance, which is a rather logical conclusion. However, it requires further investigation, which we postpone for a future work. In the case of BRR usage (right column in Figure 5.17), the bias is strongly shifted towards py.SA. It definitely may cause the performance issues due to the lack of exploration. According to presented in Figure 5.18 final results statistics, given at least one dominating LLH, HH-SP utilizes it enough times to obtain a good final solution quality.

The next setup is LLHs with tuned parameters (lower row in Figure 5.17 and right side of Figure 5.17). According to the baseline evaluation, all among available LLHs are able to tackle the problem instance producing comparable solution quality, however, the performance difference still exists (Figure 5.18). As a consequence, FRAMAB HLH learns it and frequently utilizes the best performing j.ES (lower row, middle plot in Figure 5.17). On the contrary, BRR and random-based approaches sample all LLH types evenly. We conclude that BRR is not as sensitive to the performance evidence and was 'confused', since the process quickly converged into a local optimum. The quality of all HP-SP final results presented in Figure 5.18 are at least as good, as the solution quality provided by the best underlying LLH.

**pla7397 TSP instance.** Our observations of HH-SP performance on the largest problem instance is as follows. During the baseline evaluation, py.ES with default parameters had the worst performance, while the tuned algorithm version was able to outperform only default j.ES. On the contrary, j.ES with tuned parameters produced the best results, outperforming py.SA. The best meta-heuristic with default parameters was py.SA. Therefore, we observe an expected behavior of HH-SP with default LLHs (upper row in Figure 5.19): the most frequently sampled by learning-based HLH was py.SA. However, the number of py.ES usages is suspiciously high in BRR case. Referring to the final results presented in Figure 5.20, we observe a high diversity in quality when py.ES is allocated frequently (codes 1.1. and 3.1), which is expected behavior, when the performance of py.ES with default parameters is taken into account.

Talking about the tuned LLHs usage, we observe almost equal performance of all LLH sampling approaches, comparable to the baseline results. The solution quality of random-based HLH is slightly worse, in comparison to the results of FRAMAB- and BRR-based HH-SP due to their j.ES preference (see right chart in Figure 5.20).

**Discussion.** According to our observations of the developed HH-SP performance, we conclude that the proposed concept implementation operates as expected: HH-SP provides similar to the best underlying LLH results. Two implemented selection HLH are performing slightly differently when reaching a local optimum. We claim the FRAMAB is a more perspective HLH, since it starts to balance between previously good performing LLH exposing good exploration abilities. In the cases when an advantage of one LLH changes to another, BRR may need more time to learn this.

The observed issues call not only for a thorough investigation (pla7397 code 1.1, 3.1), but also for a generic approach to handle potential flaws in the LLH implementation that may cause issues in overall execution process.

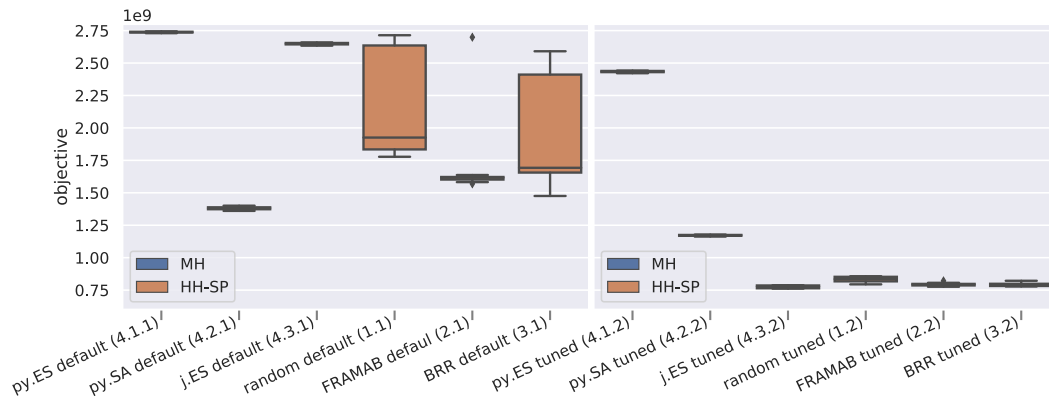
#### 5.4.5 Selection Hyper-Heuristic with Parameter Control (HH-PC)

The final evaluation is dedicated to the performance analysis of the suggested approach of merging the online selection hyper-heuristic with the generic parameter control technique. A minimal goal is to reach the best underlying LLH performance with tuned hyper-parameters. In this evaluation set we follow the used for HH-SP method of intermediate results visualization, distinguishing allocated LLH types at each iteration for single repetition. We compare the quality of final results in relation to all repetitions with a baseline using box-plots.

**kroA100, pr439 and rat783 TSP instances.** The decision of joining all three TSP instances is motivated by a similar to aforementioned reasons: the intermediate and final performance are rather similar among problem instances and do not require separate review, therefore, here we present only a single case (rat783). The results for all other problems may be found in Appendix A.1.4.

During the solving process similar to HH-SP patterns of algorithm allocation may be observed for both FRAMAB-based (codes 2.4, 2.5) and BRR (codes 3.4, 3.5) HLHs. However, in this case the intermediate results are slightly differing, since the parameter control started to search for a good LLHs configuration (Figure 5.21).

Let us firstly draw the readers' attention to HH-PC with FRAMAB-based LLH selection and TPE-based parameter sampling (code 2.4 in Figure 5.21). At the beginning of solving process, j.ES was performing



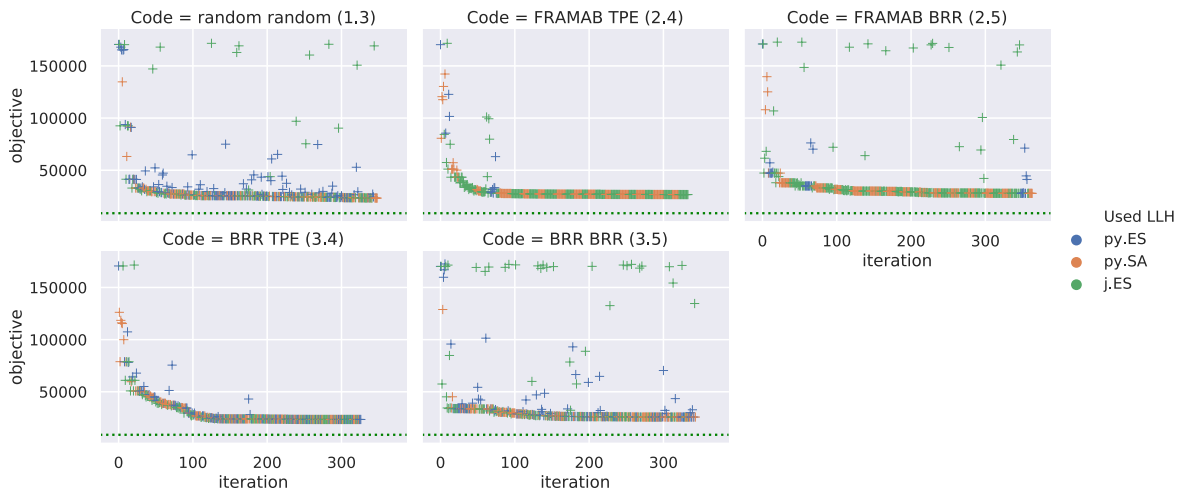
**Figure 5.20** Final results of HH-SP on pla7397 (statistic of 9 runs).



extremely well, for this reason FRAMAB was sampling it with a higher frequency. When a solving process reached its local optima (nearly 50<sup>th</sup> iteration), FRAMAB switched to exploration of the other algorithms. An appeared ‘noise’ in the results of both ES heuristics is caused by a boolean parameter *elitist*, which defines the selection strategy and may result in the solution quality degradation (more details in Section 2.2.2). From an absence of the noise in later stages of 2.4 and 3.4, we may conclude that TPE has found *elitist*=True parameter value to be perspective. On the contrary, BRR-based parameter controller did not find these parameters and glancing on the final results quality (Figure 5.22) we conclude the BRR finds statistically worse performing parameters, in comparison to TPE. Also, we must not ignore the fact of early reaching a local optimum by the search processes (see shapes of progress curves in Figure 5.21). In such case, the parameter search may be biased towards exploration. For that we need to introduce the other progress metrics, such as stagnation detection (used in EA parameter control approaches [65]) and perform multi-objective surrogate optimization, maximizing improvement and minimizing stagnation. Since it is a rather considerable amount of effort, we postpone this enhancement for the future work.

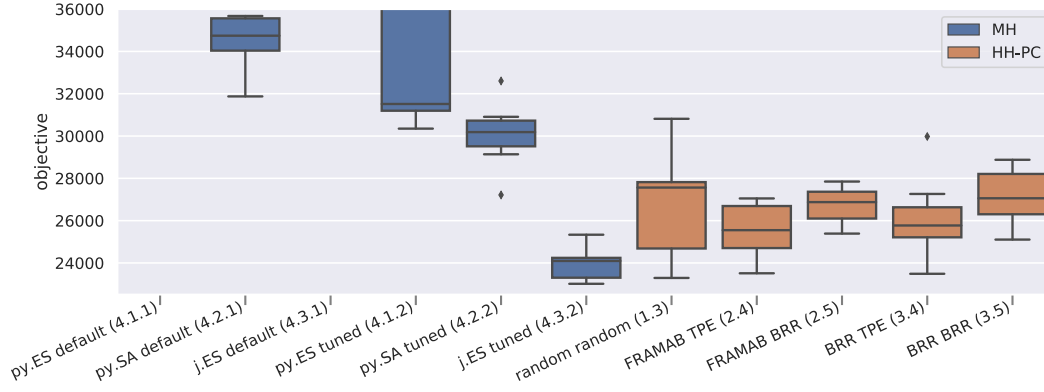
In Figure 5.22 we clearly see the dominating j.ES MH with tuned parameters (code 4.3.2). The quality of the final solution, produced by HH-PC is slightly lower than the best performing tuned j.ES. This may be explained by a lack of performance evidence obtained for the learning models, since the optimization reached its local optima too quickly.

**pla7397 TSP instance.** During these benchmarks, the issue with py.ES made a crucial change in the overall number of iterations where it was used many times (codes 1.3, 3.4, 3.5 in Figure 5.23). While the case of fully randomized HH-PC (code 1.3) is clear, a BRR LLH selection did use this LLH frequently, because it may have produced good quality solutions as a result of parameter control. On the contrary, FRAMAB LLH selection in combination with TPE parameter tuning (code 2.4) managed to find good parameters for py.SA, therefore, utilized it most often. When the FRAMABs’ exploration component weight reached critical point, the other LLHs usage was triggered and as a result, HH-PC switched to j.ES usage. This switch later gave dramatic result improvements (code 2.4 Figure 5.23). The FRAMAB LLH selection with BRR parameter control (code 2.5) at the beginning was using the mixture of mainly two j.ES and py.SA, but later switched to the simulated annealing-only usage. As we may see, it gave fast coarse-grained solution improvements at the beginning, and stable, but rather slow fine-grained improvements in the later stage.



**Figure 5.21** Intermediate performance of HH-PC on rat783 (single experiment).

## 5 Evaluation



**Figure 5.22** Final results of HH-PC compared with MH on rat783 (statistic of 9 runs).



**Figure 5.23** Intermediate performance of HH-PC on pla7397 (single experiment).

The final results quality charts (Figure 5.24) depict a dominance of FRAMAB-based LLH selection (codes 2.4, 2.5) over BRR-based and TPE-based parameter control (codes 2.4 and 3.4) over BRR-based (codes 2.5, 3.5). line, the obtained results with BRR-based parameter control are more stable than provided by TPE-surrogates. The quality of final results did not reach the best performing tuned j.ES (code 4.3.2) due to the issue with py.ES. However, since the optimization process did not settle in the local optima, we have a doubt that HH-PC will not outperform j.ES given the same number of external iterations. For a better intuition, let us draw the readers' attention to Figure 5.25. Please note, how HH-PCs are approaching j.ES progress curve. If it were not for the issue with a number of external iterations, the results would be better and, probably, outperforming the best available tuned j.ES.

**Discussion.** The observed results of tackling the united APSP problem by HH-PC are encouraging. Our approach managed to reach and in some cases even outperform the results of the best underlying LLH with tuned hyper-parameters on small problem instances (kroA100, pr439, rat783). When the problem size significantly grows (pla7397), the gap between HH-PC and the best performing LLH started to increase. An explanation for this is simple: the system needs to build surrogate models not for single, but for multiple LLHs parameters and, therefore, requires more performance evidence in comparison to MH-PC or HH-SP. line, an amount of information only decreases as a consequence of an issue with py.ES. Since the parameter values are not selected to properly reflect the LLHs performance, the algorithm

selection process also straggles. To overcome the problem with lack of information we (1) need to fix the aforementioned issue and (2) may execute an additional meta-learning step before the beginning of optimization session. An investigation of this rather intriguing idea is postponed for the future work.

#### 5.4.6 Concept Evaluation Results Discussion

We aggregate the results of each implemented mode in Tables 5.5 and 5.6. In each of them the baseline is defined as the best results obtained by the underlying meta-heuristics used separately with static parameters. As an example, the baseline for kroA100 TSP instance is defined by jMetalPy.SA with default parameters, while tuned jMetal.ES produced the best solutions for pla7397. The results for each experiment separately are presented in Appendix A.2.

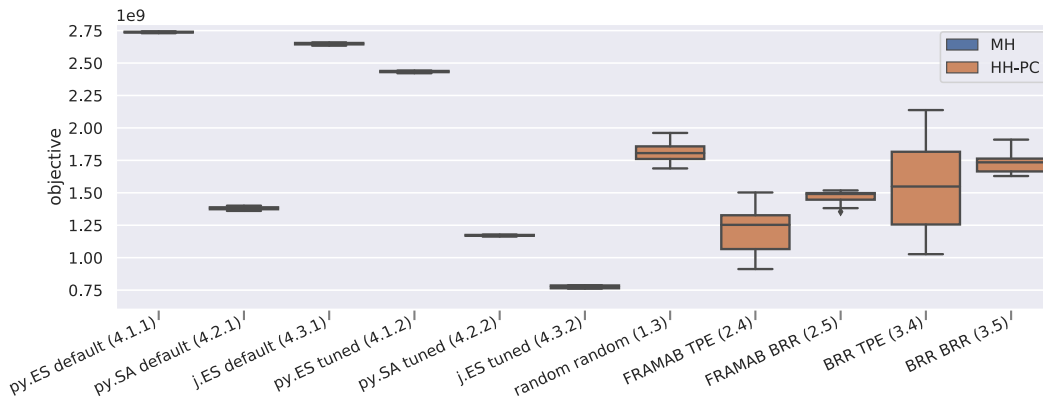
In Table 5.5 we compare the baseline with the *best* results in each mode. For instance, consider MH-PC. Statistically, the best average results for kroA100 (27178) were produced by jMetal.ES with TPE control (code 4.3.4), while the baseline is 39560. Therefore, the average result of the best MH-PC equals to 0.687 of the baseline. We perform a similar aggregation for HH-SP, excluding the experiments, where LLHs were used with tuned parameters (therefore, selecting the best among 1.1, 2.1 and 3.1 codes). As for HH-PC, we pick the best averaged results in all available experiments, for instance, on kroA100 it was code 3.4 (HH-PC with FRMAB LLH selection and TPE parameter control) with 30396 average result.

Our conclusion on Table 5.5 is as follows: if one **knows** which among available meta-heuristics statistically produces better results (with properly selected parameters), the preference is to use the proposed generic parameter control (**MH-PC**) approach.

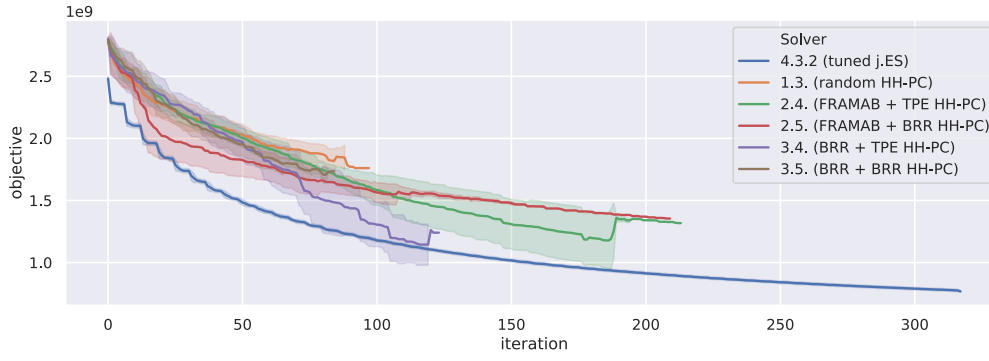
**Table 5.5** The best solution quality obtained by each mode compared with the best underlying meta-heuristic (baseline) on four TSP instances (lower is better).

TSP Instance	Baseline	MH-PC	HH-SP	HH-PC
kroA100	1	<b>0.687</b>	0.961	0.768
pr439	1	<b>0.973</b>	1.072	0.988
rat783	1	1.081	1.448	<b>1.064</b>
pla7397	1	<b>0.985</b>	2.228	1.546

However, the situation changes dramatically if one **does not know**, which meta-heuristic is the best among available. In Table 5.6 we aggregate the average results over *all* experiments in each mode. It means that the results of all meta-heuristics with parameter control are taken into account to estimate averaged MH-PC gain. However, we need to exclude several experiments to perform a fair comparison.



**Figure 5.24** Final results of HH-PC compared with MH on pla7397 (statistic of 9 runs).



**Figure 5.25** HH-PC and tuned jMetal ES solving process comparison on pla7397 (statistic of 9 runs).

**Table 5.6** Average solution quality obtained by each mode compared with the best underlying meta-heuristic (baseline) on four TSP instances (lower is better).

TSP Instance	Baseline	MH-PC	HH-SP	HH-PC
kroA100	1	0.841	0.975	<b>0.773</b>
pr439	1	1.106	1.1	<b>1.017</b>
rat783	1	2.034	1.45	<b>1.1</b>
pla7397	1	2.139	2.36	<b>1.93</b>

For MH-PC we exclude the random-based parameter selection (4.1.3, 4.2.3, 4.3.3 codes). For both HH-SP and HH-PC modes we similarly exclude the random-based LLH and parameter selection (1.1 and 1.3 codes). Also, for HH-SP we ignore the experiments with tuned in offline meta-heuristics (1.2, 2.2, 3.2).

Therefore, our conclusion for cases, when one has several meta-heuristics, but **does not know**, which is the best among them, the complex approach of simultaneous online algorithm selection and parameter tuning (**HH-PC**) should be preferred due to its strong dominance over MH-PC and HH-SP modes.

## 5.5 Analysis of HH-PC Settings

The second benchmark is dedicated to the evaluation of system settings' influence on the solving process. Due to limited time we decided to perform the parameter analysis only for the most complex system mode: online selection hyper-heuristic with parameter control in low-level heuristics (HH-PC).

### 5.5.1 Evaluation Plan

Similarly to the concept evaluation, we start this set of benchmarks from the planning. For comparison basis we selected one statistically better performing HH-PC setup, in which FRAMAB was used for the algorithm selection, and TPE for parameter control respectively. Implemented FRAMAB algorithm exposes only one hyper-parameter: the balancing coefficient  $C$ . In Section 4.3.3 we discussed its values and also proposed an approach to replace this static value by dynamically derived from results deviation. In all previous tests we used exactly this approach. TPE implementation exposes *split size* parameter, which defines the percentage of available data, used to create a distribution of good-performing parameter values (see TPE description during HpBandSter framework review in Section 2.3.2). In the previous experiments we used  $\frac{1}{3}$  of available data to construct a *good* distribution. The overall amount of information, used to construct the surrogate models was controlled by a shared parameter *window size*. In our evaluations we were using 80% of available information at each point in time. As one may

remember, we did not implement an elegant algorithm for surrogates optimization, but used the random search instead to select the best parameter set by means of their results on surrogates. Thus, we used a predefined number (96, the default value in BRISv2) of randomly sampled parameter values on each level (more details in Section 4.3.3). Also, our setup included 6 workers and task execution time was set to 15 seconds. The implemented RL approach implies the iterative solving process, therefore, the workers were sending a complete bunch of obtained solutions to main node after accomplishing a task. All aforementioned characteristics form three groups of experiments:

1. **Learning granularity** group is designed to investigate the influence of performance evidence amount and quality to optimization process. It is formed by such parameters as *window size*, *task time* and *number of workers*.
2. **Learning models configuration** group of experiments is dedicated to investigate the influence of HLH parameters on the quality of the results and includes *FRAMAB C coefficient*, *TPE split size* and *random search size*.
3. **Amount of warming-up information** is a self-describing experiment, dedicated to investigate an influence of warming-up solutions numbers to initialize LLH at each external iteration.

We define the estimation values for the proposed parameters in Table 5.7.

**Table 5.7** Prediction techniques used for the concept evaluation.

Parameter	Investigated values	Default value
<i>Learning granularity</i>		
Window size	30%, 50%, 100%	80%
Task time	5, 10, 30 seconds	15 seconds
Number of workers	3, 9, 12	6
<i>Learning models configuration</i>		
TPE split size	10%, 50%, 70%	30%
FRAMAB C coefficient	Static 0.001, 0.01, 0.1	STD-based
Random search size	50, 200	96
<i>Amount of warming-up information</i>		
Warming-up solutions	one	all

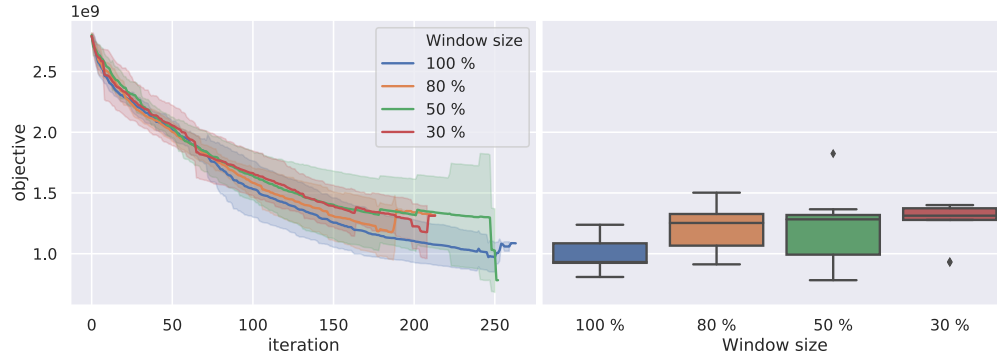
We set all other parameters as they were configured during HH-PC evaluation: the experiment running time is set to 15 minutes, the number of experiment repetitions is 9 and the search space is unchanged.

The idea of performing the full factorial design was quickly abandoned, since it requires 46 days of non-stop experiment running. Therefore, the performed one-exchange benchmark design resulted in 18 experiments, which needed 40,5 hours to perform 9 repetitions.

### 5.5.2 Learning Granularity

In this experiment we investigate the influence of RL routines configuration on learning process. The idea is as follows. Changing the *window size*, *task time* and *number of workers*, the underlying surrogate models may learn a different dependencies picture. For instance, if we increase a task time, each sampled configuration will be measured more thoroughly, however, given the same experiment running time, the overall number of iteration will be decreased. On the contrary, by increasing a number of workers, a portion of investigated APSP space will be increased, therefore, the underlying learning models will construct more precise surrogates.

**Please note**, the perturbations at the end of progress charts are caused by the same issue with the number of performed iterations, discussed in Section 5.4.2.

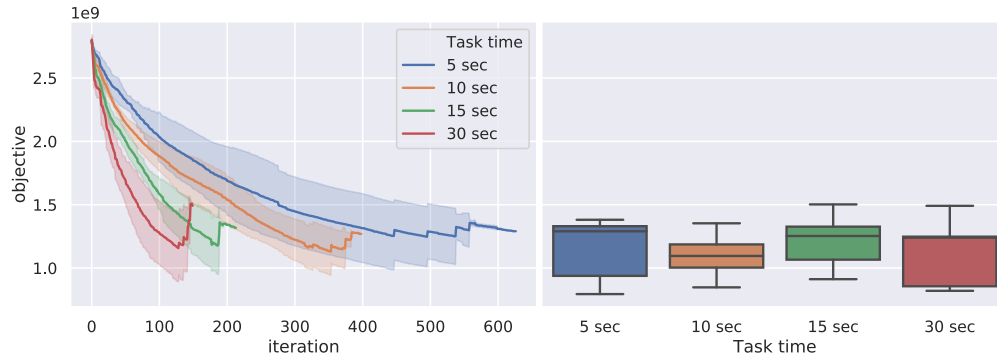


**Figure 5.26** Influence of HH-PC (code 2.4) window size on pla7397 TSP instance solving process.

**Window size.** According to our expectations in Section 3.3, this parameter is responsible for the forgetting mechanism, which is required to follow possibly changing trends in optimization process.

In Figure 5.26 we presented the results obtained with four different window sizes. We observe that the best results are obtained, when the learning models were used all the available information, in other words, with disabled forgetting mechanism. On the contrary, with the smallest window size the quality of final results is expectedly the worst. A trend could be observed, according to which HH-PC provides a better quality of results with larger window size. In our previous benchmarks we were using 80% of the available information, which corresponds to the middle-quality parameter value.

Our conclusion is the following: with this problem instance and system setup, changes in the learning process and parameter preference are mostly negligible, therefore, the forgetting mechanism should be disabled. In the future, it would be rather intriguing to investigate this parameter influence on other, potentially dynamic problem instances.

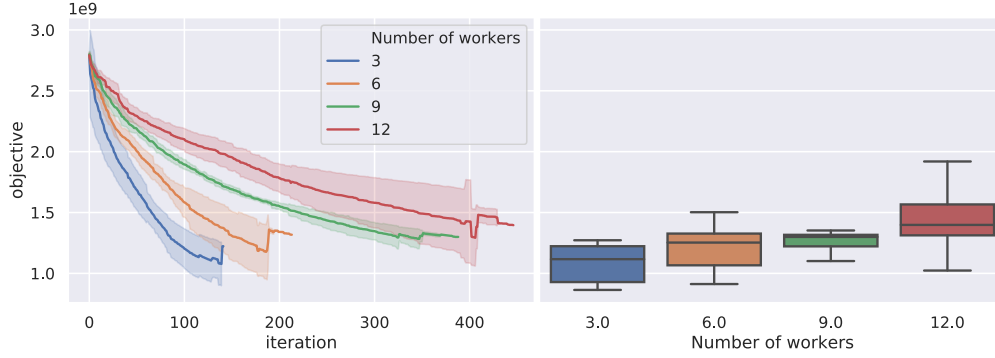


**Figure 5.27** Influence of HH-PC (code 2.4) task time on pla7397 TSP instance solving process.

**Task time.** Varying the time for one task evaluation (external iteration), one will dramatically change the granularity of obtained results. For instance, in our experiments with the least task time (5 seconds) HH-PC performed more than 600 external iterations, while with the largest budgeted (30 seconds), this number was approximately 150 (Figure 5.27). As we previously observed, more information does not necessarily imply better surrogate models creation. Used during the concept evaluation 15 seconds task time provided the worst results. Boundary cases of 5 and 30 seconds of task time gave rather unstable results (see box-plots in Figure 5.27). The former is full of too approximately evaluated parameters, while the later simply did not manage to perform enough iterations. Balancing between results stability and quality, we conclude that for the current setup statistically better choice would be to set a task



running time equal 10 seconds.



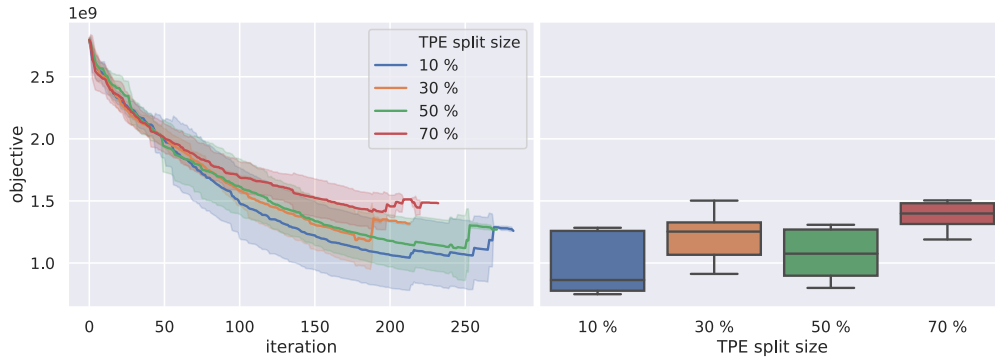
**Figure 5.28** Influence of HH-PC (code 2.4) workers number on pla7397 TSP instance solving process.

**Number of workers.** The influence of workers' number was a surprise to us. According to our expectations, with a growing number of LLH runners, the proportion of estimated parameter space increases. However, instead of getting better quality surrogate models and, as a result, improving sampled parameters performance, we observe the opposite behavior. For increasing number of workers the results became worse and worse (see box-plots in Figure 5.28). Currently, we do not have a comprehensive explanation of the observed behavior, except for the possible surrogate models over-fitting. It is a broadly studied problem in the ML field, according to which the model learns too complex hypothesis, which cannot generalize well to unforeseen data. Thus, in our case it is possible that being over-fitted, surrogates did not adequately predict results for sampled parameters and, therefore, guided prediction process in a wrong direction. In any case, this behavior requires more comprehensive investigation in the future work.

### 5.5.3 Learning Models Configuration

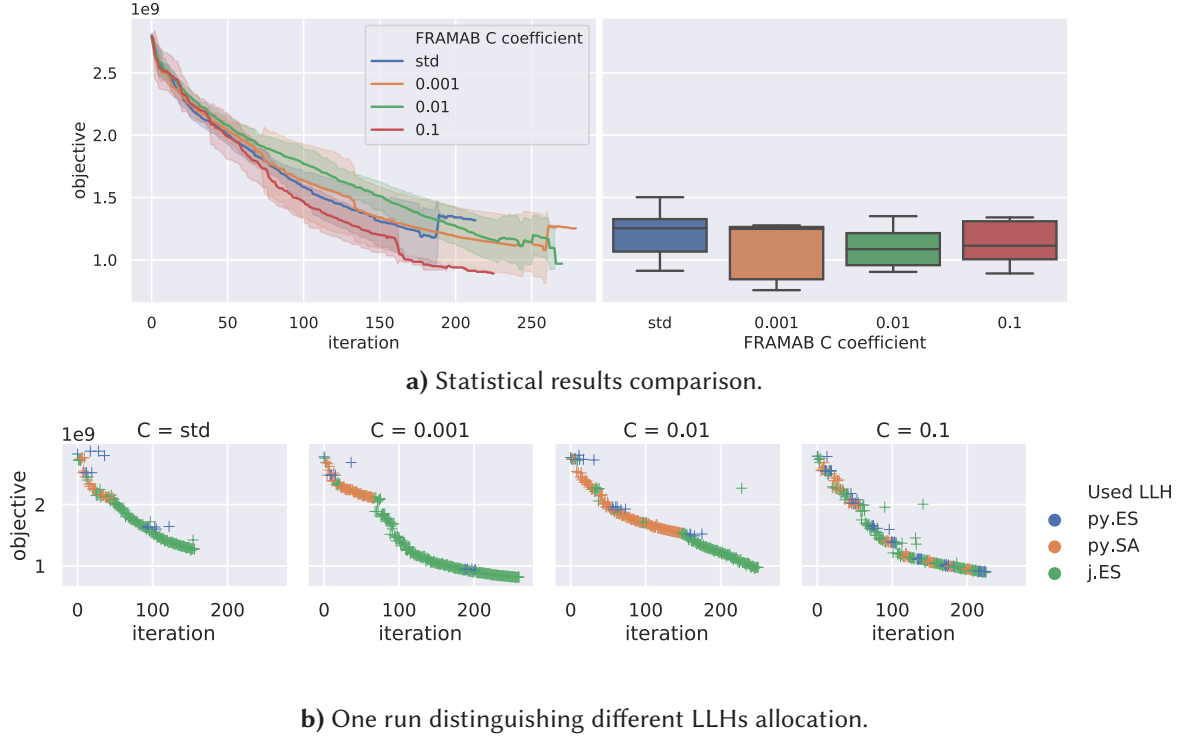
We perform this set of experiments for getting an intuition about the underlying high-level heuristic configuration influence on a general performance.

**TPE split size.** The internals of Bayesian TPE approach for parameter sampling were described in Section 2.3.2. With small split size, only elite parameter values form a *good* distribution, therefore, an overall sampling process happens to be more greedy or, in other words, biased towards exploitation. According to our observations, visualized in Figure 5.29, the more greedy parameter allocation produces statistically better results (10%), while usage of 70% split showed the worst potential.



**Figure 5.29** Influence of HH-PC (code 2.4) TPE split size on pla7397 TSP instance solving process.

## 5 Evaluation



**Figure 5.30** Influence of HH-PC (code 2.4) FRAMAB C coefficient on pla7397 TSP instance solving process.

**FRAMAB C coefficient.** As the reader remembers from FRAMAB description, presented in Section 4.3.3, the role of coefficient  $C$  is to control the EvE balance while selecting the LLH. In our implementation we proposed to replace  $C$  with the improvements standard deviation, therefore, in first set of benchmarks we exclusively used this, STD-based FRAMAB regime.

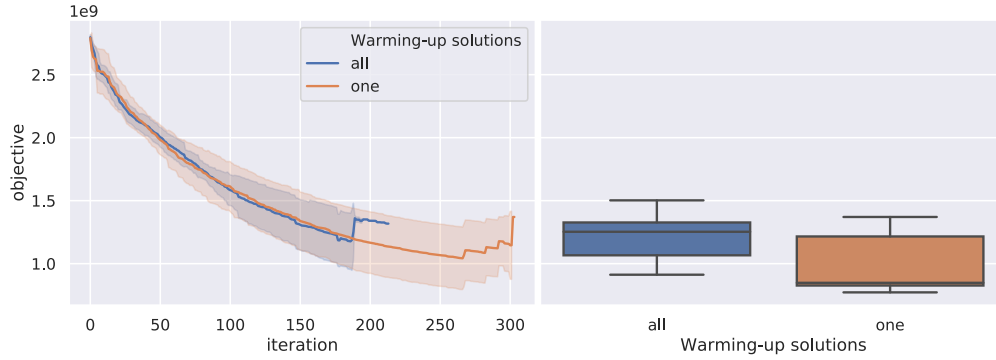
The results of performed benchmarks with different  $C$  values are presented in Figure 5.30. More concretely, in Figure 5.30a we compare statistics of all repetitions with different parameter values. We conclude, the proposed parameter-less (STD-based) FRAMAB version produces similar results in comparison to other cases. When  $C$  (or STD) is large, the exploration-related component of FRAMABs' UCB value is increased, therefore, more different algorithms are used for optimization. However, when the  $C$  value is decreased, only several switches may be observed (Figure 5.30b). An intriguing idea arises to introduce the technique for FRAMAB parameter control, according to which, the entire LLH portfolio is utilized at the beginning with high  $C$  value, while approaching the end  $C$  is increased to concentrate on the best-performing LLH.

**Random search size.** This HLH parameter configures the random search process, performed over the created surrogate models. According to our expectations, the increased random search size should result in a more precise parameter values prediction and as a consequence, to performance gain. However, evaluating random search sizes of 50 and 200 samples respectively, the obtained results happen to be not as we expected. In general, we observe a quality fluctuation, which is caused by the randomized processes. It only motivates us to implement a proper surrogate optimization technique for improving a robustness of the prediction process.



**Figure 5.31** Influence of HH-PC (code 2.4) random search size for surrogate optimization on pla7397 TSP instance solving process.

#### 5.5.4 Amount of Warming-up Information



**Figure 5.32** Influence of HH-PC (code 2.4) warming-up solution number on pla7397 TSP instance solving process.

Here we evaluate how the *number of warming-up solutions* affects the search. Our intuition during the implementation was following: we should initialize the solver with all previously obtained solutions not to lose the derived optimization trajectory and traversal velocity. However, it is relevant only to the population-based algorithms, such as evolution strategy or potential genetic algorithm.

After changing this behavior to only one warming-up solution usage, we surprisingly found out that the quality of the results was almost not affected: please, pay attention to overlapping progress curves in a left side of Figure 5.32. Moreover, by passing only one solution between LLHs we dramatically increased the overall number of external iterations (for more than 50%). It is caused by the reduced overhead for information processing and sending through the network. We conclude that changing the behavior to only one warming-up solution usage provides a positive impact on the quality of the final results and does not affect the intermediate performance of meta-heuristics.

## 5.6 Conclusion

The evaluation of proposed concept was presented in this Chapter and performed in two stages. At the first stage an analysis of the implemented concept applicability was performed. We compared it with a baseline, defined by the executed in isolation underlying meta-heuristics with static hyper-parameters. Our conclusions on the concept applicability are following:

- Firstly, the proposed reinforcement learning-based generic parameter control approach (MH-PC)

is able to significantly improve the performance of meta-heuristics' static hyper-parameters and in some cases even outperform the quality of tuned at the design time parameters.

- Secondly, the developed heuristic selection technique (HH-SP) is able to reach a quality of the best performing underlying low-level heuristic.
- Finally, the approach for simultaneous online algorithm selection and parameter tuning (HH-PC) outperforms the best underlying algorithm with tuned parameters on rather small problem instances (kroA100, pr439). With growing complexity, HH-PC only approaches the quality of the best available algorithm with tuned parameters.

Our conclusions on the implemented concept usage are the following: when the dominance among meta-heuristics is known beforehand, one should consider the MH-PC usage with this MH; if the dominance is not known, but the parameters of meta-heuristics are already tuned (which may be rare use-case), one should consider HH-SP usage; but if the dominance of MHs is not known and proper parameter values are unknown as well, one should naturally utilize the proposed HH-PC concept to tackle the optimization problem at hand.

In the second part of evaluation we investigated the HH-PC configuration influence on its performance. The impact of some among evaluated parameters was not as we expected, which only motivates the importance of a proper parameter values search and usage. More concretely, an insertion of the relatively light *forgetting mechanism* instead of improving only made the results statistically slightly worse. The increased number of workers only decreased surrogate models accuracy. The decision on all available solutions usage for LLH initialization introduced a redundant overhead, but did not improve final results quality, therefore, it should be reconsidered. Nevertheless, a set of experiments from the second evaluation stage should also be performed over the other system operating modes (MH-PC and HH-SP) and problem instances. By doing so, we will be able to make a confident conclusion about the stability and impact of different parameter values. Up until now, it revealed the system adaptation ability with help of exposed parameters and helped us find several incorrect decisions.

## 6 Conclusion

Before making a final conclusion, let us briefly remind our objective. The task of this thesis was defined as follows: using an existing parameter tuning software proposes a concept to (1) perform the parameter control in meta-heuristics on a generic level and (2) make both algorithm selection and parameter control solve the optimization problem at hand. In our research the complex objective was split into several compound tasks, which were formulated in three research questions (Section 1.2). Here we provide explicit answers to each of them.

The proposed in this thesis generic parameter control approach relies on two aspects. Firstly, it should be possible to evaluate the performance of the system under control with specified configuration at any time. The ideal option is to limit the system execution with the budget specified beforehand (number of iterations, wall-clock time, etc). Secondly, it should be possible to change the target algorithm configuration and proceed with the execution basing on previously obtained results. We use the reinforcement learning methodologies to traverse the parameter space, evaluating the performance of unforeseen configurations iteratively, while solving the problem at hand. The proposed concept of generic parameter control was examined in Section 5.4.3 with three meta-heuristics: two Python-based algorithms, namely, simulated annealing and evolution strategy and one Java-based evolution strategy. The proposed approach revealed its applicability by reaching, and in some cases even outperforming the results of tuned in offline algorithm parameters. Therefore, we answer the **RQ1**: it is indeed possible to perform the algorithm configuration at runtime on the generic level. Please note, the use-cases of our concept are defined by the algorithms, in which execution time is much larger than time spent to parameter control routines (see Section 3.1).

**RQ2** *Is it possible to simultaneously perform algorithm selection and parameters adaptation while solving an optimization problem?*

Our idea of merging those two problems lays in treating the algorithm type as a regular categorical parameter in the search space. By utilizing the parent-child relationships we define dependent parameters in such search space and perform the selection by means of firstly sampling the independent parameters and hiding the children, and secondly fixing the selected for parents' values and exposing the *activated* children parameters. The proposed stepwise process of configuration construction provides a possibility to utilize a wide range of surrogate models for learning the dependencies among parameter values on each level in isolation. The requirements and use-cases of the proposed approach remain the same as for the generic parameter control technique defined above.

**RQ3** *What is the effect of selecting and adapting algorithms while solving an optimization problem?*

The performed in Section 5.4.5 evaluation and analysis of the simultaneous online algorithm selection and parameter control revealed its applicability. More specifically, given the same wall-clock time and environment setup, HH-PC was able to outperform the best underlying tuned meta-heuristics for kroA100 TSP instance. For a slightly larger pr439 example, HH-PC results were comparable with the best tuned in offline meta-heuristic. With problem size growing further, the gap between HH-PC and the best available solver, used in isolation with tuned parameters increases. However, comparing the averaged quality of all available solvers used in isolation with the results of our approach, we observe a strong

domination of later. Therefore, our answer to **RQ3** is the following: HH-PC constantly produces good quality results and should be considered if the meta-heuristics domination and their hyper-parameters are unknown beforehand. However, a considerable amount of solution quality is sacrificed to tackle APSP problem, in comparison to the best underlying algorithm usage with tuned parameters.

An explicit list of this thesis contributions is the following:

1. The concept of reinforcement learning-based generic parameter control in meta-heuristics was proposed and empirically evaluated.
2. The unification of both online algorithm selection and generic parameter control approaches into single APSP is performed. The approach to tackle APSP is proposed by means of reinforcement learning-based online selection hyper-heuristic with parameter control in low-level meta-heuristics.
3. The usability of an existing parameter tuning SPL BRISv2 was extended with aforementioned use-cases without losing the flexibility of a wide range of learning models usage. Moreover, the concept of data preprocessing was encapsulated.

We consider the task of this thesis accomplished and the proposed reinforcement learning-based generic parameter control and algorithm selection approaches useful for solving the optimization problems with the help of meta-heuristics.



## 7 Future Work

In this chapter we discuss the investigations, postponed for future work. We organized them into several groups and sort each of them in the descendant order by means of urgency and importance. Section 7.1 is dedicated to the prediction process and learning models used in HLH of developed approach. In Section 7.2 we discuss a set of enhancements for the search space that should be performed for better usability. Finally, in Section 7.3 we discuss benchmark experiments, required to obtain better evidence about the proposed approach applicability and HH-PC in particular.

### 7.1 Prediction Process

**Surrogate optimization generalization.** In Section 4.3 we discussed the process of parameter values prediction based on surrogate models. A classical approach of optimization with surrogates implies two steps. Firstly, the models should be constructed and evaluated by means of their accuracy. If the model is not accurate enough, it could result in a wrong prediction and as a consequence in wrong optimization guidance. After getting a proper model, the second step should be performed, namely, surrogate optimization. It is an actual process of prediction making, which is based on construction of configuration and using surrogate to estimate its quality. In our work we used a random search surrogate optimization technique instead of implementing a more sophisticated algorithm due to the lack of time. However, the evaluation of random search intensity (Figure 5.31) revealed the urgency of this question, since the quality of random search results is not stable. Therefore, one of the first steps in future work should be the implementation of proper algorithm for surrogate model optimization.

**Process metrics for reinforcement learning.** The proposed concept of reinforcement learning-guided parameter space traversal is based on the estimation of relative improvement, performed by the selected parameters (Section 3.1). However, the amount of obtained information may not be enough to truly estimate the configuration quality. We would like to emphasize that it is not a problem of the surrogates, but of the reinforcement learning. Thus, the possible improvement of results may be obtained from adding additional RL metrics. For instance, a RL-based parameter control for EAs [65] besides algorithm-dependent metrics, such as genotypic and phenotypic diversity, fitness standard deviation (in population) used also algorithm-independent metrics such as fitness improvement and stagnation counter. While improvement estimation is already used in our concept, the later, namely, a stagnation estimation is a possible candidate for additional learning metrics. Please note, using several such metrics, the surrogate optimization process turns to be a multi-objective OP.

**Meta-/offline learning phase.** Relying fully on the online learning, in early stages (while surrogate models cannot be constructed properly due to lack of information) our concept behaves like a random search. However, many studies somehow related to proposed technique reported a significant performance boost in early stages, if the offline or in other words meta-learning was performed. More specifically, in [44] (also discussed in Section 2.4) the authors performed meta-learning to pre-train their surrogate models for guiding the search at the beginning. In [115] the authors developed selection hyper-heuristic with mixed learning type, therefore, before an actual run, the offline phase was executed

to guide the online selection at early stages. In our system we could use the results of previously executed experiments for similar scenario case to guide right from the start not only the LLH selection, but also the parameter control.

Separately we would like to highlight a recent study [13], in which the authors also suggest to use reinforcement learning approach to solve a similar *dynamic algorithm configuration* problem. In their work the problem was enclosed in Markov decision processes, which include meta-learning step: learning across the problem instances.

## 7.2 Search Space

**Composition on numerical parameters.** In current implementation of the search space we highlight that it is able to form the parent-child relationship only when parent is of the categorical type (Section 4.2.2). However, it may happen, when the dependencies among parameters are based on their numeric values. As an example, imagine the algorithm in which for one parameter values range the first child type should be exposed, while for the other range — another child. As a possible solution we propose utilizing an approach, similar to the one used in categorical parameters, but instead of a single activation value, use ranges. Thus, during the prediction propagation step the parameter entity will check all ranges and expose the related children (for more details see description of the Listing 4.6).

**Constraints among parameters.** Sometimes, the prohibitions for specific values may arise with respect to other parameters. For instance, the value of one numeric parameter should be at least as high as the value of the other. In this case, along with activation values the notion of deactivation values may be introduced.

## 7.3 Evaluations and Benchmarks

The presented in Chapter 5 evaluation contains only the coarse-grained set of experiments, however, the proposed in this thesis concept of merging algorithm selection and parameter control comprises several building blocks, each of which should be thoroughly evaluated separately. Therefore, here we propose a set of fine-grained directions for future evaluation.

### 7.3.1 Use-Case Evaluation

**Optimization problems.** The advantage of hyper-heuristics lays in their ability to tackle a *family* or *class* of optimization problems, defined by underlying low-level heuristics. Due to this flexibility of hyper-heuristics in general and the proposed concept in particular, by changing the domain-dependent components of low-level heuristics one will be able to tackle numbers of other optimization problems. Our evaluation in Chapter 5 is performed only on a traveling salesman problem. However, the combinatorial problems also include other types such as *flow-shop scheduling* [53], *nurse rostering* [26], *knapsack* [99], *n-queens* [97] and many other real-life and synthetic optimization problems. Used in our implementation jMetalPy framework [6] out of the box includes domain-dependent components for aforementioned knapsack problem, but thanks to its flexibility it is relatively easy to add other problem types.

**Construction hyper-heuristics.** The idea discussed in Section 2.2.5 of construction hyper-heuristics implies the algorithm creation from the building blocks. In our work we treated the *mutation*, *crossover*, *selection types* as the categorical parameters of underlying LLHs. However, in used jMetal and jMetalPy frameworks these parameters are implemented as separate operators that should be specified during

the algorithm instantiation. Therefore, the proposed concepts of search space and RL-based parameter assignment may be evaluated also for the construction hyper-heuristic cases.

**Automatic machine learning.** Making a step further from construction hyper-heuristic, an orthogonal research direction of an automatic machine learning field is exposed. The framework reviewed in Section 2.4 deals with the construction of machine learning pipelines that operate on datasets. In our approach, the proposed representation of the search space may be used to define the ML pipeline structure. For instance, the first several levels of our search space may encode the data preprocessing in ML pipeline. The successive level denotes the ML algorithm instances, while the final level is dedicated to validation technique. This system use-case should be evaluated against the already proposed solutions in automatic machine learning field, for instance, AutoSklearn [44], TPOT [88] and many others.

### 7.3.2 System Configuration Evaluation

The benchmark set, presented in Section 5.5 is dedicated to the implemented concept configuration evaluation. Due to the time constraints, we were able to probe only a few system modes and settings. Nevertheless, a vast bunch of experiments should be conducted urgently.

**Modes of operation.** In Section 5.5 only to HH-PC mode was benchmarked. However, it includes two other modes, namely MH-PC and HH-SP, which configuration should be evaluated separately by means of (1) underlying surrogate models settings, (2) adding more LLHs. While the influence of the first direction was partially relieved in Section 5.5, the second direction, which is relevant only to HH-SP and HH-PC modes requires more clarification. By extending the search space with more LLHs, the RL will require more information (in terms of external iterations) for tuning available LLHs and differentiating among them by means of their performance. It is clear that with LLH number growth, the final performance gap between the best performing (tuned) LLH and HH-PS (HH-PC) will increase. The goal of these experiments will lay in a dependency estimation between search space complexity and the introducing RL-based search overhead.

**Reinforcement learning configuration.** Another worth-to-mention course of investigation is the influence of currently implemented RL-based optimization approach. The experiments with different TSP instances showed inefficiency of strictly defined time-based external iterations. For instance, with kroA100 TSP most of the used LLHs reached the local optimum after a couple of first external iterations and settled there till the end of optimization process. Thus, the *adaptive external iteration time* should be introduced, which analyze the process stagnation and thus, be able to terminate the optimization session earlier.

On the contrary, instead of time-based mechanism for external iteration termination, one may also limit the number of internal iterations performed by LLH. Using this mechanism the set of use-cases may be extended, with the expensive for evaluation optimization problems.



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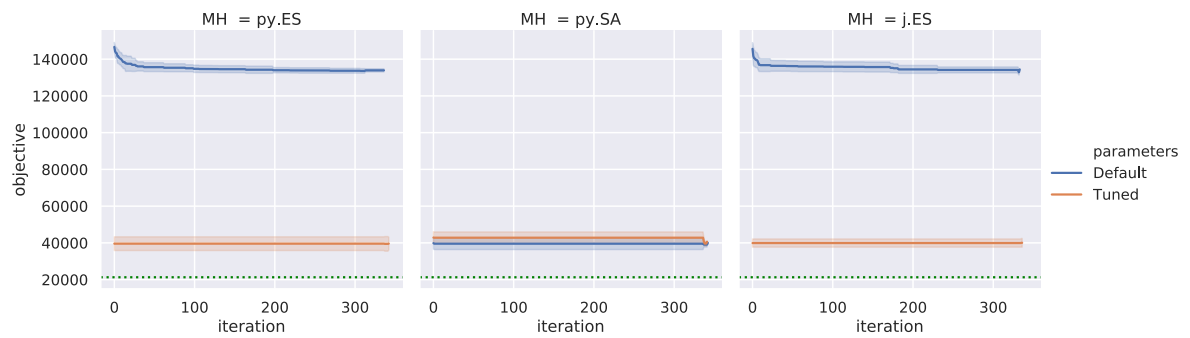
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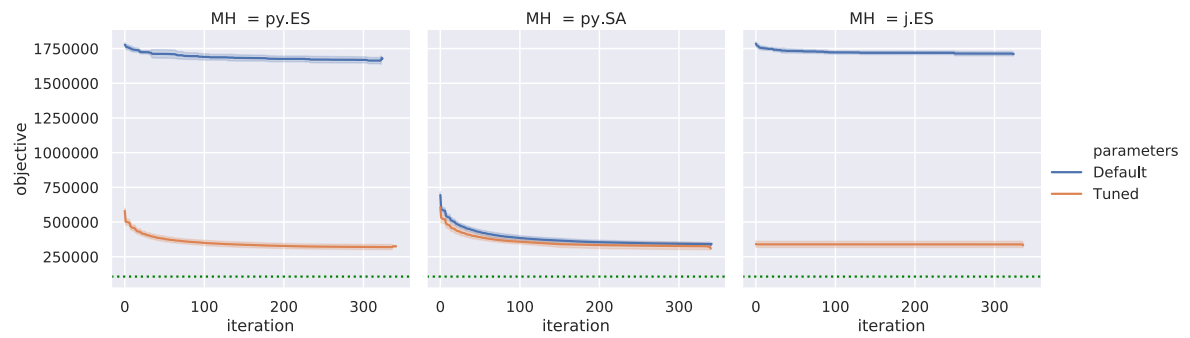
# A Evaluation Results

## A.1 Results in Figures

### A.1.1 Baseline

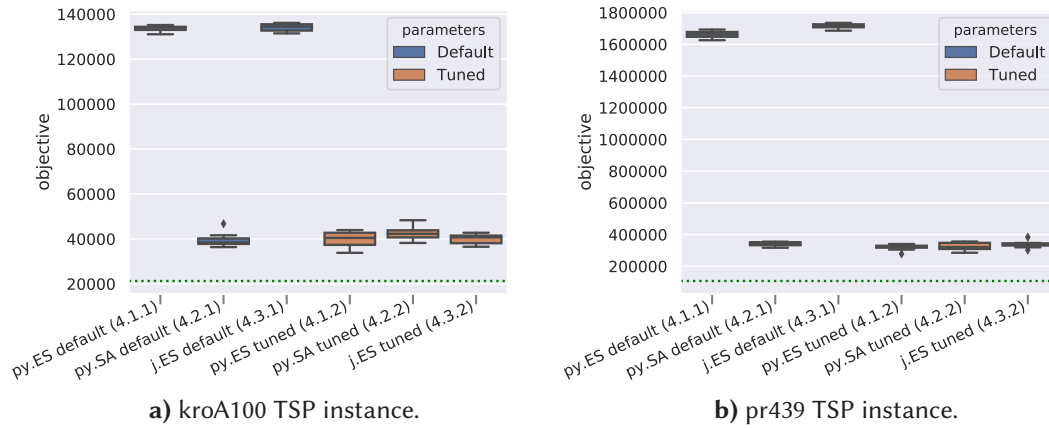


**Figure A.1** Intermediate results of meta-heuristics with static parameters on kroA100.



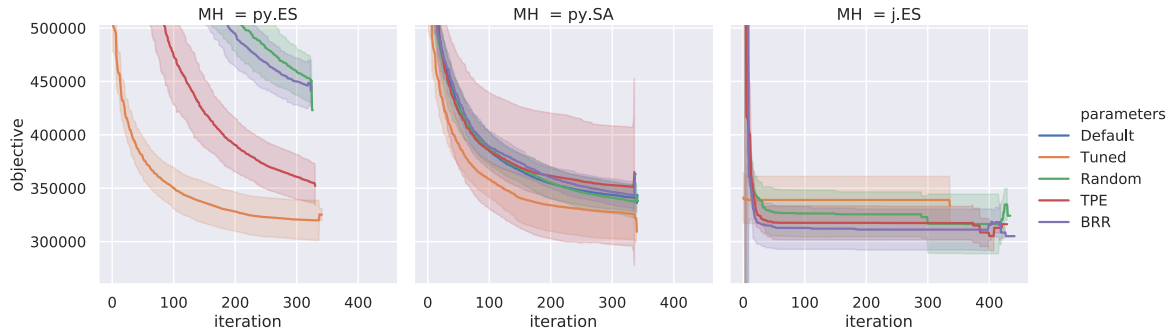
**Figure A.2** Intermediate results of meta-heuristics with static parameters on pr439.

## A Evaluation Results

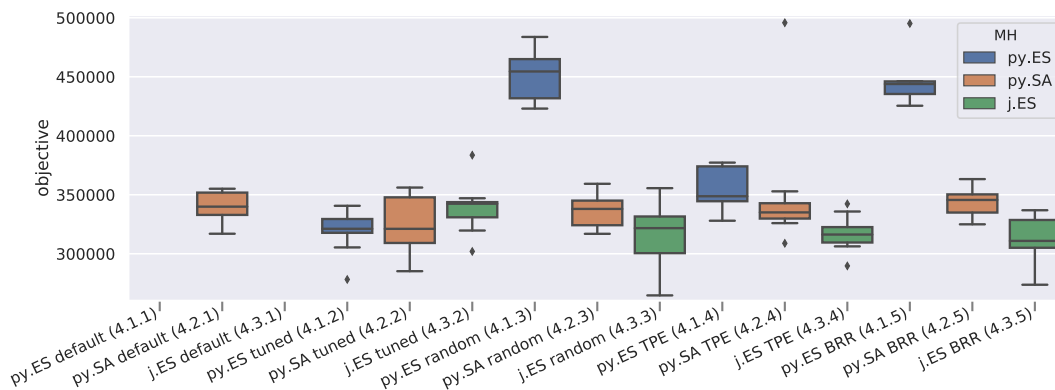


**Figure A.3** Final results of meta-heuristics with static parameters.

### A.1.2 Parameter Control



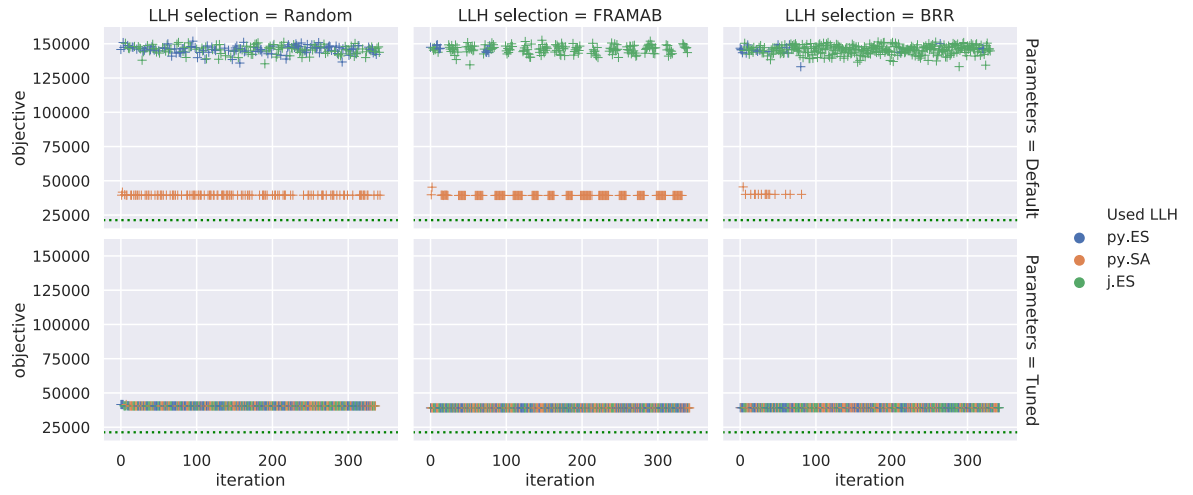
**Figure A.4** Intermediate results of meta-heuristics with parameter control on pr439.



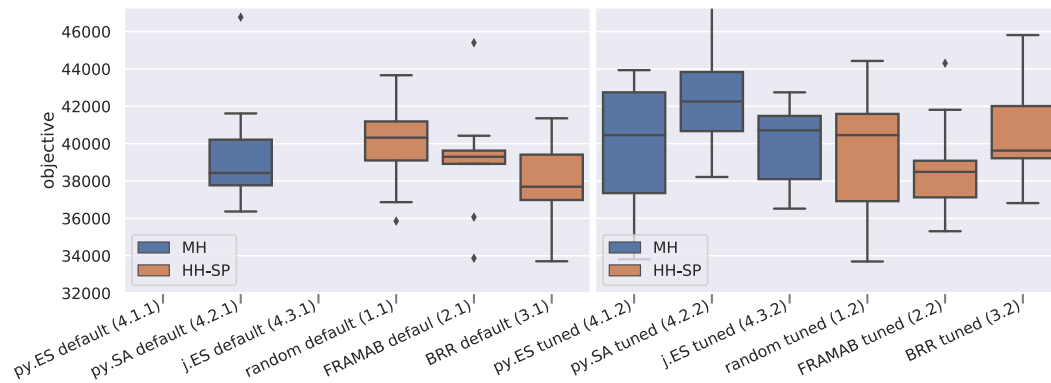
**Figure A.5** Final results of meta-heuristics with parameter control on pr439.

### A.1.3 Selection Hyper-Heuristic with Static LLH Parameters



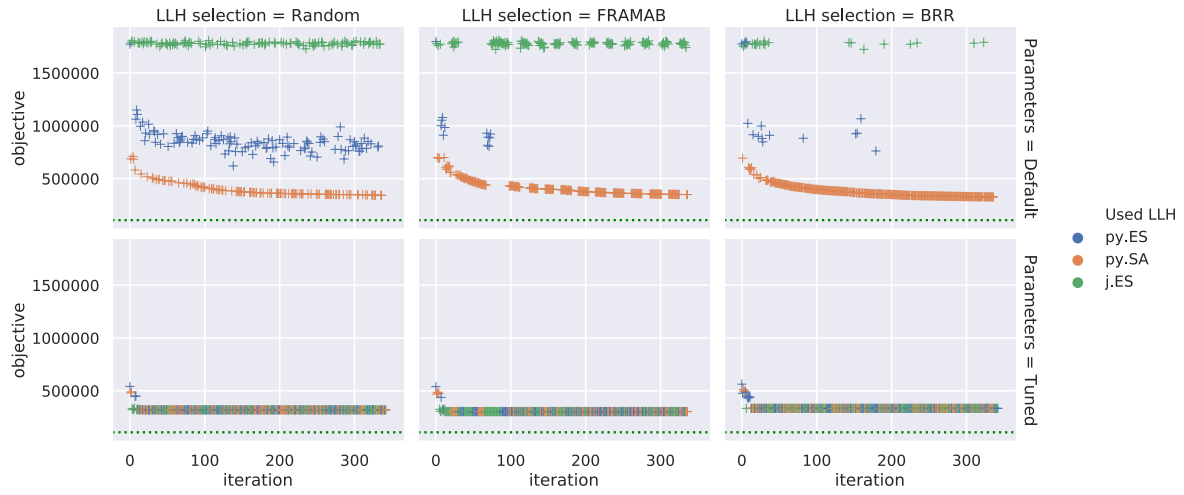


**Figure A.6** Intermediate performance of on-line selection hyper-heuristic with static hyper-parameters on kroA100 (single experiment).

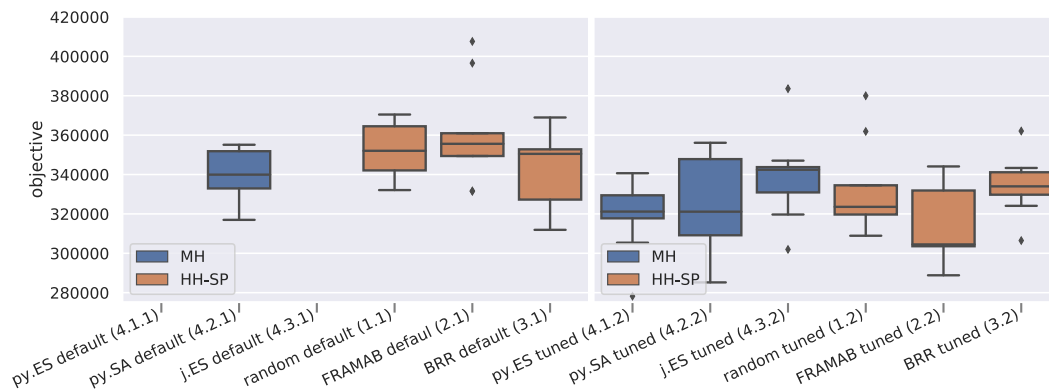


**Figure A.7** Final results of on-line selection hyper-heuristic with static hyper-parameters on kroA100 (statistic of 9 runs).

## A Evaluation Results



**Figure A.8** Intermediate performance of on-line selection hyper-heuristic with static hyper-parameters on pr439 (single experiment).



**Figure A.9** Final results of on-line selection hyper-heuristic with static hyper-parameters on pr439 (statistic of 9 runs).

## A.1.4 Selection Hyper-Heuristic with Parameter Control

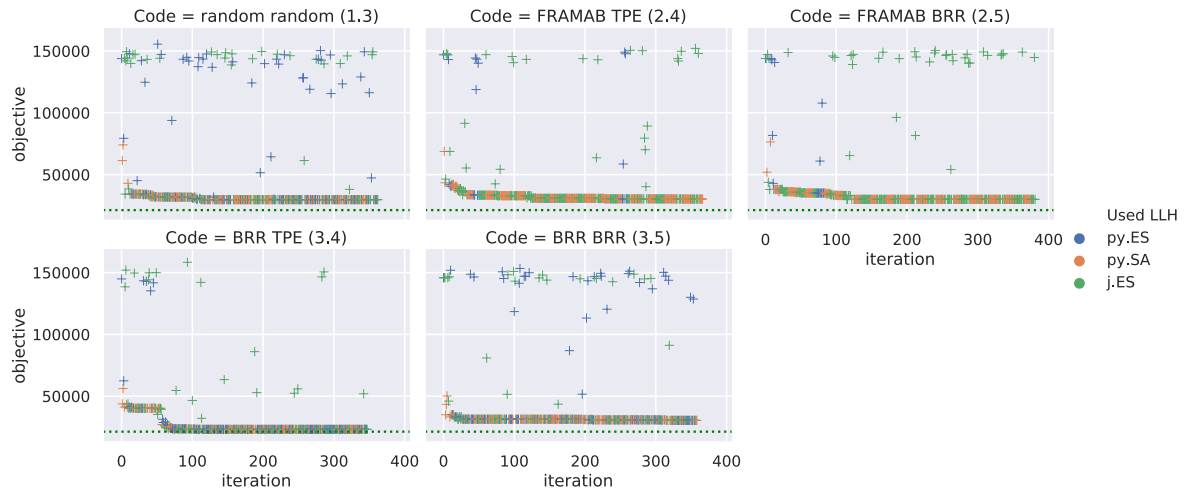


Figure A.10 Intermediate performance of HH-PC on kroA100 (single experiment).

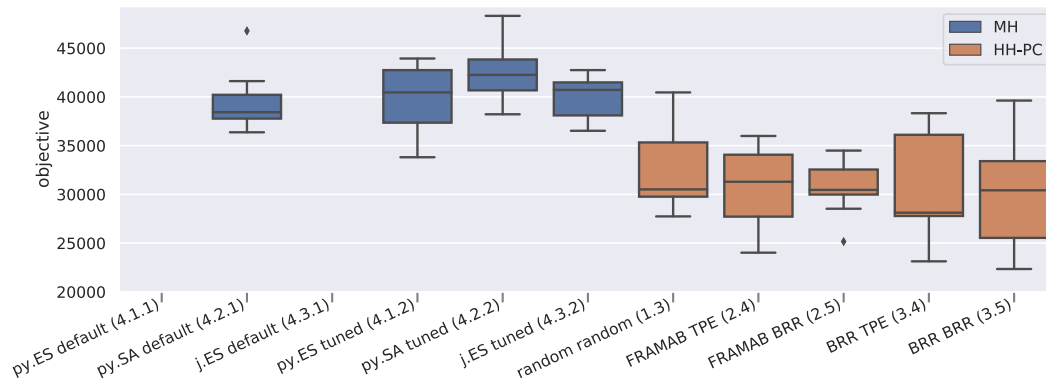
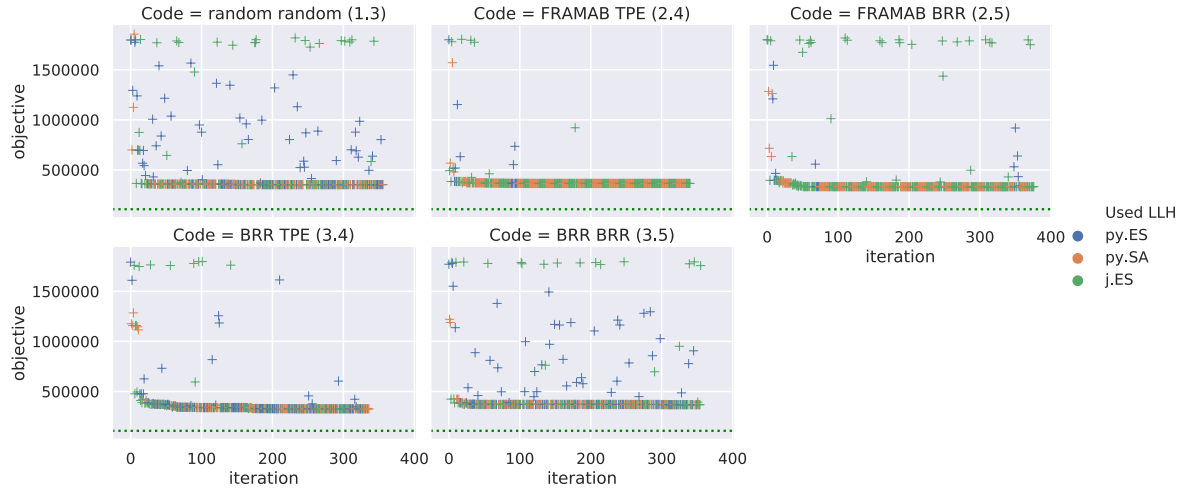
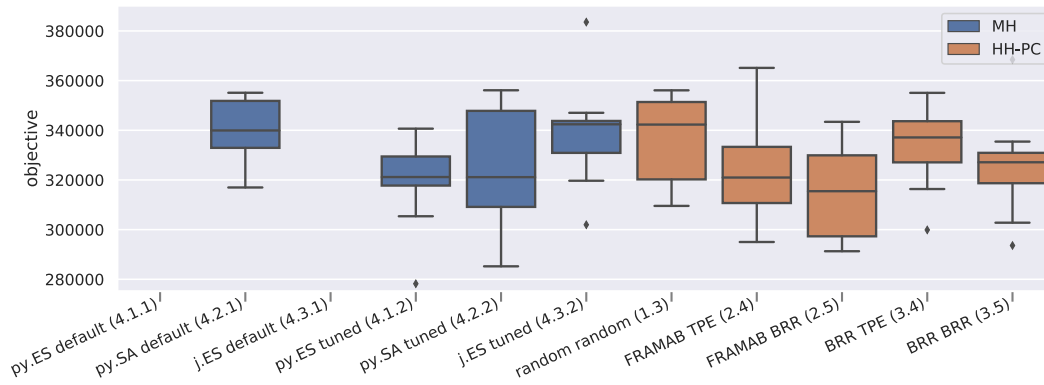


Figure A.11 Final results of HH-PC compared with MH on kroA100 (statistic of 9 runs).

## A Evaluation Results



**Figure A.12** Intermediate performance of HH-PC on pr439 (single experiment).



**Figure A.13** Final results of HH-PC compared with MH on pr439 (statistic of 9 runs).

## A.2 Results in numbers

**Table A.1** Found paths distances for kroA100 TSP instance (optimal path length is 21282). The best result in experiment group is highlighted in bold, while the best result found for problem instance is also underscored.

Solver		Results		
Group	Code	Best found	Average	STD
Baseline	4.1.1	131075	133596	1249
	4.1.2	<b>33809</b>	39572	3738
	4.2.1	36368	<b>39560</b>	3191
	4.2.2	38216	42819	3149
	4.3.1	131453	134141	1634
	4.3.2	36522	39905	2242
MH-PC	4.1.3	33160	35219	1760
	4.1.4	27563	35265	4836
	4.1.5	31223	34790	2727
	4.2.3	34902	37986	2548
	4.2.4	32264	37145	3008
	4.2.5	31481	36497	3575
	4.3.3	24415	29768	5202
	4.3.4	<b>23855</b>	<b>27178</b>	1851
	4.3.5	24567	28793	3209
HH-SP	1.1	35853	40057	2585
	1.2	<b>33692</b>	39261	3431
	2.1	33868	39135	3132
	2.2	35312	38920	2711
	3.1	33704	<b>38019</b>	2237
	3.2	36818	40461	2565
HH-PC	1.3	27741	32404	4133
	2.4	24019	30652	3958
	2.5	25160	30764	2869
	3.4	23132	<b>30396</b>	5407
	3.5	<b>22345</b>	30564	5826

**Table A.2** Found paths distances for pr439 TSP instance (optimal path length is 107217). The best result in experiment group is highlighted in bold, while the best result found for problem instance is also underscored.

Solver		Results		
Group	Code	Best found	Average	STD
Baseline	4.1.1	1625689	1663522	22427
	4.1.2	<b>278214</b>	<b>319803</b>	18705
	4.2.1	316973	340823	12546
	4.2.2	285220	325721	23970
	4.3.1	1685919	1713684	14766
	4.3.2	301964	338969	22113
MH-PC	4.1.3	423043	450570	20626
	4.1.4	327995	354661	18535
	4.1.5	425453	445088	20507
	4.2.3	316908	337100	15007
	4.2.4	308850	351326	55555
	4.2.5	324957	343358	12607
	4.3.3	<u>264713</u>	316496	27886
	4.3.4	289704	317360	15600
HH-SP	4.3.5	273744	<b>311078</b>	19442
	1.1	332095	351533	13784
	1.2	308913	332514	24001
	2.1	331487	360533	25971
	2.2	<b>288830</b>	<b>313859</b>	19735
	3.1	311906	342915	19211
HH-PC	3.2	306461	334998	15175
	1.3	309552	334987	18995
	2.4	295015	324616	21519
	2.5	<b>291299</b>	<b>315932</b>	18866
	3.4	299884	333992	17465
	3.5	293607	325887	21150



**Table A.3** Found paths distances for rat783 TSP instance (optimal path length is 8806). The best result in experiment group is highlighted in bold, while the best result found for problem instance is also underscored.

Solver		Results		
Group	Code	Best found	Average	STD
Baseline	4.1.1	150799	156314	4157
	4.1.2	30350	39203	12357
	4.2.1	31873	35157	2825
	4.2.2	27215	30094	1393
	4.3.1	164349	165617	644
	4.3.2	<b>23015</b>	<u>23964</u>	724
MH-PC	4.1.3	57003	94429	49422
	4.1.4	38223	78434	59507
	4.1.5	62964	96369	48767
	4.2.3	32459	34229	1305
	4.2.4	30335	31545	749
	4.2.5	31475	33691	1784
	4.3.3	<b>23607</b>	26183	1353
	4.3.4	24517	<b>25916</b>	952
	4.3.5	25202	26450	796
HH-SP	1.1	34490	36637	1132
	1.2	23341	24233	741
	2.1	33029	34794	1444
	2.2	<u>22816</u>	24324	1007
	3.1	32006	34693	1507
	3.2	22927	<b>24149</b>	797
HH-PC	1.3	<b>23292</b>	26921	2430
	2.4	23512	<b>25500</b>	1334
	2.5	25388	26721	908
	3.4	23488	26129	1801
	3.5	25105	27114	1233

**Table A.4** Found paths distances for pla7397 TSP instance (optimal path length is 23260728). The best result in experiment group is highlighted in bold, while the best result found for problem instance is also underscored.

Solver		Results		
Group	Code	Best found	Average	STD
Baseline	4.1.1	2730074917	2737831472	4225616
	4.1.2	2421486544	2432905011	7405688
	4.2.1	1360505168	1380256720	13657387
	4.2.2	1162583357	1171728906	5239671
	4.3.1	2633785765	2648540705	8181262
	4.3.2	<b>761509264</b>	<b>775957737</b>	10846169
MH-PC	4.1.3	2729415229	2738113236	7383459
	4.1.4	2712114799	2734298124	9381522
	4.1.5	2723433962	2732529772	5694368
	4.2.3	1354022277	1369131424	11698311
	4.2.4	1186230750	1407196180	292371422
	4.2.5	1255612025	1271166341	14802252
	4.3.3	933923318	1109347363	85835240
	4.3.4	<b>663489188</b>	<b>764140101</b>	108747262
HH-SP	4.3.5	903993065	1048196489	109819327
	1.1	1777658580	2203819260	437999367
	1.2	794461798	832754319	22848007
	2.1	1569150086	1728591281	364476875
	2.2	<b>775887027</b>	794478412	13501812
	3.1	1475527859	1934187052	449660041
HH-PC	3.2	777931654	<b>791768317</b>	14578963
	1.3	1687855495	1815721794	87307521
	2.4	<b>912264049</b>	<b>1199738016</b>	205533985
	2.5	1354196166	1460681037	57770764
	3.4	1026880309	1579805637	375451837
	3.5	1629147332	1736442893	89413787

## **Confirmation**

I confirm that I independently prepared the thesis and that I used only the references and auxiliary means indicated in the thesis.

Dresden, 11th May 2020