



# Metaheuristic Optimization in Python: moptipy

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# Outline

1. Introduction
2. Log Files in moptipy
3. Repeatability and Replicability
4. Parallel and Distributed Runs
5. Summary
6. Advertisement





# Introduction



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- We here discuss how such features can be achieved.



# Log Files in moptipy





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  8. the system configuration, including processor, memory, Operating System (OS), library versions..., and
  9. exceptions and the stack trace if something went wrong.

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- No complicated format like JavaScript Object Notation (JSON), YAML Ain't Markup Language™ (YAML), or Extensible Markup Language (XML)! (Makes parsing complex. Different people may use different subsets of their functionality.)

# moptipy Log File Structure

```
BEGIN_PROGRESS  
fes;timeMS;f  
1;6;267  
5;7;235  
10;7;230  
20;7;227  
25;7;205  
40;7;200  
84;8;180  
END_PROGRESS
```

**Progress of the Algorithm over Time**  
fes ... consumed objective function evaluations  
timeMS ... consumed runtime in milliseconds  
**f** ... objective value of the fes-th evaluated solution  
Here, only moves improving the best-so-far solution are logged.  
The 10th solution that was evaluated had objective value 230. Its evaluation was completed 7ms after the begin of the run.

```
BEGIN_STATE  
totalFEs: 84  
totalTimeMillis: 8  
bestF: 180  
lastImprovementFE: 84  
lastImprovementTimeMillis: 8  
END_STATE
```

**End State at the end of the optimization run**  
total consumed FEs  
total consumed runtime in milliseconds (ms)  
best objective value encountered  
FE when the last improvement took place  
ms when the last improvement took place

```
BEGIN_SETUP
```

**Algorithm and Problem Instance Information**  
p.name: LoggingProcessWithSearchSpace  
p.class: moptipy.api.\_process\_ss\_log.\_ProcessSSLog  
p.lowerBound: 180  
p.upperBound: 482  
p.maxTimeMillis: 120000  
p.goalF: 180  
p.randSeed: 6526669205530947346  
p.randSeedHex: 0x5a9363100a272f12  
p.randGenType: numpy.random.\_generator.Generator  
p.randBitGenType: numpy.random.\_pcg64.PCG64  
a.name: rls\_swap2  
a.class: moptipy.algorithms.so.rls.RLS  
a.op0.name: shuffle  
a.op0.class: moptipy.operators.permutations.  
 op0\_shuffle.Op0shuffle  
a.op1.name: swap2  
a.op1.class: moptipy.operators.permutations.op1\_swap2.Op1Swap2  
y.name: gant\_demo  
y.class: moptipy.examples.jssp.gantt\_space.GanttSpace  
y.shape: (5, 4, 3)

algorithm name  
algorithm class  
nullary operator

unary operator

solution space setup

```
y.dtype: h  
y.inst.name: demo  
y.inst.class: moptipy.examples.jssp.instance.Instance  
y.inst.machines: 5  
y.inst.jobs: 4  
y.inst.makespanLowerBound: 180  
y.inst.makespanUpperBound: 482  
y.inst.dtype: b  
f.name: makespan  
f.class: moptipy.examples.jssp.makespan.Makespan  
f.lowerBound: 180  
f.upperBound: 482  
x.name: perm4w5r  
x.class: moptipy.spaces.permutations.Permutations  
x.nvars: 20  
x.dtype: b  
x.min: 0  
x.max: 3  
x.repetitions: 5  
g.name: operation_based_encoding  
g.class: moptipy.examples.jssp.  
    ob_encoding.OperationBasedEncoding  
g.dtypeMachineIdx: b  
g.dtypeJobIdx: b  
g.dtypeJobTime: h  
END_SETUP
```

**BEGIN\_SYS\_INFO** Information about the System Running the Experiment

```
session.start: 2023-06-20 04:51:52.514777+00:00  
session.node: home  
session.procId: 0x3d08  
session.cpuAffinity: 4;5  
session.ipAddress: 192.168.1.109  
version.Pillow: 9.4.0  
version.contourpy: 1.0.6  
version.cycler: 0.11.0  
version.fonttools: 4.38.0  
version.joblib: 1.2.0  
version.kiwisolver: 1.4.4  
version.llvmlite: 0.40.0
```

versions of libraries used

```
version.matplotlib: 3.7.1  
version.moptipy: 0.9.76  
version.numba: 0.57.0  
version.numpy: 1.24.3  
version.packaging: 21.3  
version.pdfo: 1.3.1  
version.psutil: 5.9.5  
version.pyParsing: 3.0.9  
version.pythondateutil: 2.8.2  
version.scikitLearn: 1.2.2  
version.scipy: 1.10.1  
version.six: 1.16.0  
version.threadpoolctl: 3.1.0  
hardware.machine: x86_64  
hardware.nPhysicalCpus: 8  
hardware.nLogicalCpus: 16  
hardware.cpuMhz: (2200MHz..3700MHz)*16  
hardware.byteOrder: little  
hardware.cpu: AMD Ryzen 7 2700X Eight-Core Processor  
hardware.memSize: 33595326464  
python.version: 3.10.6 (main, May 29 2023, 11:10:38) ~  
    [GCC 11.3.0]  
python.implementation: CPython  
os.name: Linux  
os.release: 5.19.0-45-generic  
os.version: 46-22.04.1-Ubuntu SMP PREEMPT_DYNAMIC Wed Jun 7  
15:06:04 UTC 20  
END_SYS_INFO
```

**BEGIN\_RESULT\_X** Best Encoded Solution (if any)

```
2;1;3;1;0;0;2;0;1;2;3;1;0;2;1;3;0;3;2;3  
BEGIN_RESULT_Y Best Discovered Point in the Solution Space  
1;20;30;0;30;40;3;145;2;170;180;1;0;20;0;40;60;2;60;80;3;16  
5;180;2;0;30;0;60;80;1;80;130;3;130;145;1;30;60;3;60;90;0;90;13  
0;2;130;170;3;0;50;2;80;92;1;130;160;0;160;170  
END_RESULT_Y
```

information about system hardware

Python interpreter infos

operating system information



# Repeatability and Replicability



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- No other source of randomness allowed.
- The seeds  $s$  should be chosen fairly (no cherry picking possible) and in a well-defined, reproducible manner.

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- Draw unsigned 64-bit integers as seeds  $s$  alternatingly from  $\mathfrak{R}_1$  and  $\mathfrak{R}_2$  until  $n$  unique values have been collected.

# Advantages of this Method

- Random seeds are generated by a deterministic and replicable procedure.



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  - Different algorithm performance will truly be due to the different decisions that the algorithms make, not a fluke due to different starting points...
- Different seeds for different instances avoids always using the same seeds, increases fairness.



# Parallel and Distributed Runs



# File and Directory Structure

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- One directory “`results/name( $\mathcal{A}$ )`” is created for each algorithm setup  $\mathcal{A}$ , whereas  $\mathcal{A}$  is user-defined, e.g., it could be “`rls_flip1`” for randomized local search (RLS) with a single-bit-flip operator.

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A screenshot of a file explorer window titled "dmu67". The left pane shows a tree view of the directory structure:

- results
- 1rs
- ea\_1\_1\_swap2
- ea\_1\_2\_swap2 (selected)
- abz8
- dmu67 (selected)
- dmu72
- la38
- orb06
- swv14
- ta70
- yn4
- ea\_1\_4\_swap2
- abz8
- dmu67
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The right pane displays a list of files with their names, dates modified, and preview icons:

Name	Date modified
ea_1_2_swap2_dmu67_0x1bf185ca856fb9...	2022-08-24 00:47
ea_1_2_swap2_dmu67_0x3d2c1c4217421...	2022-08-24 00:31
ea_1_2_swap2_dmu67_0x6ce80008c43df3...	2022-08-24 00:45
ea_1_2_swap2_dmu67_0x6e4604d8f8396...	2022-08-24 00:35
ea_1_2_swap2_dmu67_0x8a1b06738a2b7...	2022-08-24 00:11
ea_1_2_swap2_dmu67_0x8d9e461038cc7...	2022-08-24 00:07
ea_1_2_swap2_dmu67_0x71b9eeb1e3822...	2022-08-24 00:41
ea_1_2_swap2_dmu67_0x73a895a8f6c77...	2022-08-24 00:17
ea_1_2_swap2_dmu67_0x118a344d47263...	2022-08-24 00:39
ea_1_2_swap2_dmu67_0x209f853091658...	2022-08-24 00:23
ea_1_2_swap2_dmu67_0x386aa7d0573c7...	2022-08-24 00:37
ea_1_2_swap2_dmu67_0x4173987473b57...	2022-08-24 00:03
ea_1_2_swap2_dmu67_0xae41a9b8323fd...	2022-08-24 00:25
ea_1_2_swap2_dmu67_0xb5c731b7901ca...	2022-08-24 00:15
ea_1_2_swap2_dmu67_0xb21dd40850968...	2022-08-24 00:43
ea_1_2_swap2_dmu67_0xbc8ccf94f0cfb7...	2022-08-24 00:21
ea_1_2_swap2_dmu67_0xceae54e2b92bb...	2022-08-24 00:29
ea_1_2_swap2_dmu67_0xdadb5cf502b3b...	2022-08-24 00:33
ea_1_2_swap2_dmu67_0xdfad2d5722fbe...	2022-08-24 00:13
ea_1_2_swap2_dmu67_0xfaf66f2d09...	2022-08-24 00:05

23 items

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- ⇒ We have a clearly defined directory structure for experimental results.
- ⇒ If the random seeds  $s$  are generated deterministically, then the same experiment will always yield the exactly same file names and directory structure *and* the file contents will also be the same (with the exception of stored clock time measurements, of course).

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- Otherwise, we perform the run, collect all information in memory, and write it to the log file after the run completes.

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- The state is always clear: If a log file has non-zero size, the corresponding run has completed. Otherwise, it crashed.
- Since random seeds, log files, and their locations are deterministic, starting the same experiment twice will do the same runs and produce the same log files (skipping all completed runs. . . ).

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- No inter-process communication, no exchange of data, no mutexes, no job queues, no synchronization . . . the file system takes care of everything for us.

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- It also offers implementation and benchmark datasets of many the classical  $\mathcal{NP}$ -hard tasks from Operations Research (OR).
- If you are developing new algorithms, it is quite an ideal testbed to explore your methods!



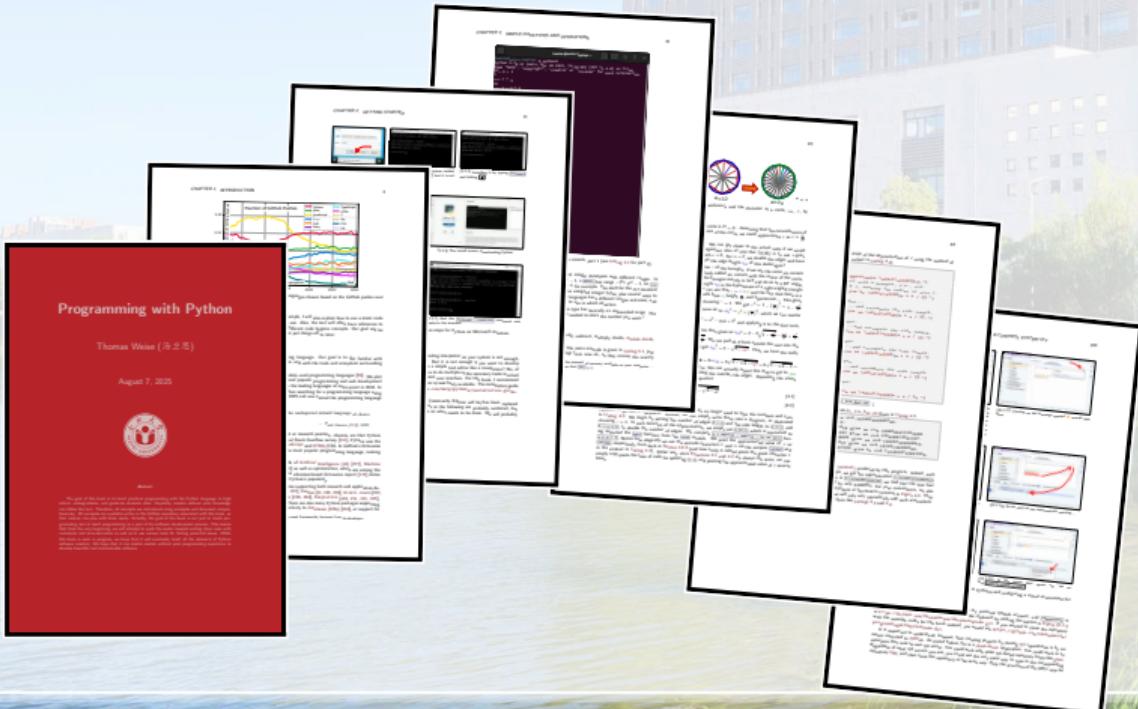
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# Programming with Python



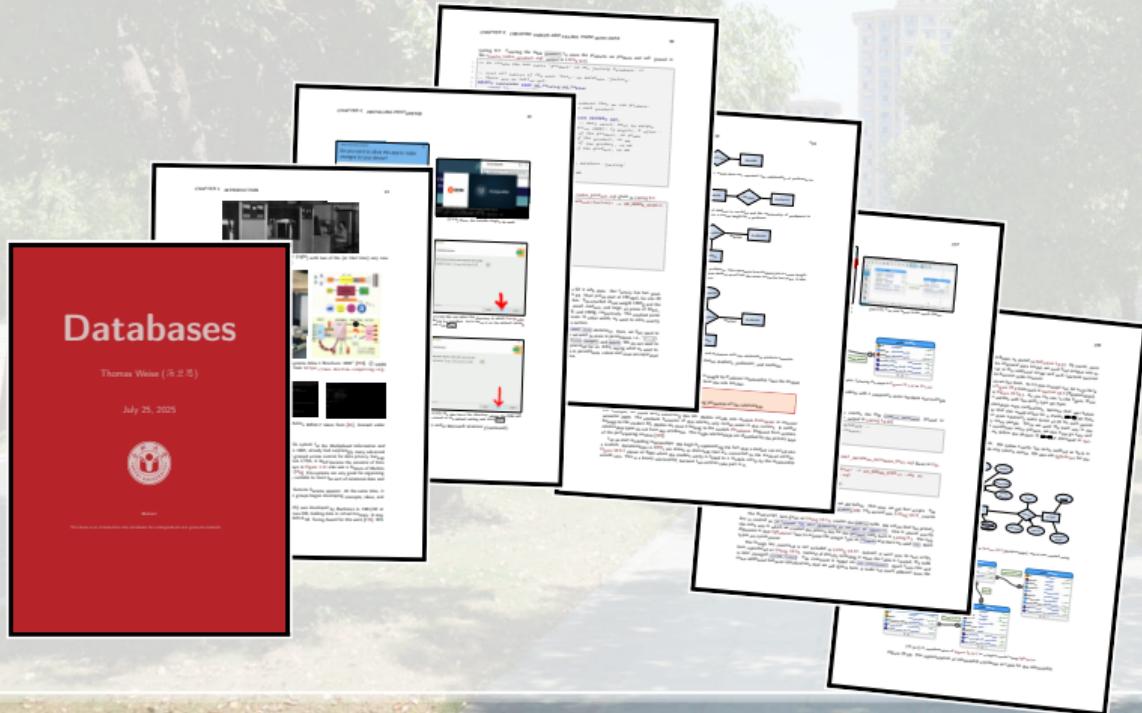
We have a freely available course book on *Programming with Python* at <https://thomasweise.github.io/programmingWithPython>, with focus on practical software development using the Python ecosystem of tools<sup>66</sup>.



# Databases

We have a freely available course book on *Databases* at

<https://thomasweise.github.io/databases>, with actual practical examples using a real database management system (DBMS)<sup>63</sup>.



# Metaheuristic Optimization in Python: moptipy

We offer moptipy<sup>69</sup> a mature open source Python package for metaheuristic optimization, which implements several algorithms, can run self-documenting experiments in parallel and in a distributed fashion, and offers statistical evaluation tools.



The screenshot shows a web browser with several tabs open, illustrating the documentation and experimental features of moptipy:

- Top Tab:** moptipy: Metaheuristic Optimizer - [moptipy.readthedocs.io/en/latest/index.html](#)
- Second Tab:** moptipy: Metaheuristic Optimizer - [thomasweise.github.io/moptipy/](#)
- Third Tab:** moptipy 0.9.148 documentation - [thomasweise.github.io/moptipy/](#)
- Fourth Tab:** moptipy: Metaheuristic Optimization in Python - [thomasweise.github.io/moptipy/](#)
- Fifth Tab:** moptipy: Metaheuristic Optimization in Python - [thomasweise.github.io/moptipy/](#)
- Sixth Tab:** moptipy: Metaheuristic Optimization in Python - [thomasweise.github.io/moptipy/](#)
- Seventh Tab:** moptipy: Metaheuristic Optimization in Python - [thomasweise.github.io/moptipy/](#)
- Content Area:** The main area displays the moptipy documentation, starting with the Table of Contents and the Introduction section. It includes code snippets, screenshots of command-line interfaces, and progress plots.





谢谢您们！  
Thank you!  
Vielen Dank!



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# Glossary I

- (1 + 1) EA The (1 + 1) EA is a local search algorithm that retains the best solution  $x_c$  discovered so far during the search<sup>9,20</sup>. In each step, it applies a unary search operator to this best-so-far solution  $x_c$  and derives a new solution  $x_n$ . If the new solution  $x_n$  is *better or equally good* when compared with  $x_c$ , i.e., not worse, then it replaces it, i.e., is stored as the new  $x_c$ . If the search space are bit strings of length  $n$ , then the (1 + 1) EA uses a unary search operator that flips each bit independently with probability  $m/n$ , where usually  $m = 1$ . This operator is the main difference to randomized local search (RLS). The (1 + 1) EA is a special case of the  $(\mu + \lambda)$  evolutionary algorithm ( $(\mu + \lambda)$  EA) where  $\mu = \lambda = 1$ .
- EA An *evolutionary algorithm* is a metaheuristic optimization method that maintains a population of candidate solutions, which undergo selection (where better solutions are chosen with higher probability) and reproduction (where mutation and recombination create a new candidate solution from one or two existing ones, respectively)<sup>2,64</sup>.
- $(\mu + \lambda)$  EA The  $(\mu + \lambda)$  EA is an evolutionary algorithm (EA) where, in each generation,  $\lambda$  offspring solutions are generated from the current population of  $\mu$  parent solutions. The offspring and parent populations are merged, yielding  $\mu + \lambda$  solutions, from which then the best  $\mu$  solutions are retained to form the parent population of the next generation. If the search space is the bit strings of length  $n$ , then this algorithm usually applies a mutation operator flipping each bit independently with probability  $1/n$ .

Android is a common operating system for mobile phones<sup>54</sup>.

CSV *Comma-Separated Values* is a very common and simple text format for exchanging tabular or matrix data<sup>52</sup>. Each row in the text file represents one row in the table or matrix. The elements in the row are separated by a fixed delimiter, usually a comma (","), sometimes a semicolon (";"). Python offers some out-of-the-box CSV support in the `csv` module<sup>16</sup>.

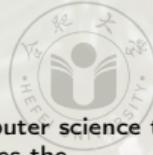
DB A *database* is an organized collection of structured information or data, typically stored electronically in a computer system. Databases are discussed in our book *Databases*<sup>63</sup>.

DBMS A *database management system* is the software layer located between the user or application and the database (DB). The DBMS allows the user/application to create, read, write, update, delete, and otherwise manipulate the data in the DB<sup>74</sup>.



# Glossary II

- JavaScript** JavaScript is the predominant programming language used in websites to develop interactive contents for display in browsers<sup>22</sup>.
- JSON** *JavaScript Object Notation* is a data interchange format<sup>6,56</sup> based on JavaScript<sup>22</sup> syntax.
- JSSP** The *Job Shop Scheduling Problem*<sup>4,35</sup> is one of the most prominent and well-studied scheduling tasks. In a JSSP instance, there are  $k$  machines and  $m$  jobs. Each job must be processed once by each machine in a job-specific sequence and has a job-specific processing time on each machine. The goal is to find an assignment of jobs to machines that results in an overall shortest makespan, i.e., the schedule which can complete all the jobs in the shortest time. The JSSP is  $\mathcal{NP}$ -complete<sup>10,35</sup>.
- Linux** is the leading open source operating system, i.e., a free alternative for Microsoft Windows<sup>3,26,53,59,61</sup>. We recommend using it for this course, for software development, and for research. Learn more at <https://www.linux.org>. Its variant Ubuntu is particularly easy to use and install.
- macOS** or Mac OS is the operating system that powers Apple Mac(intosh) computers<sup>49,55</sup>. Learn more at <https://www.apple.com/macos>.
- Microsoft Windows** is a commercial proprietary operating system<sup>5</sup>. It is widely spread, but we recommend using a Linux variant such as Ubuntu for software development and for our course. Learn more at <https://www.microsoft.com/windows>.
- moptipy** is the *Metaheuristic Optimization in Python* library<sup>69</sup>. It has been used in several different research works, including<sup>11,38–40,58,73,76,77</sup>. Learn more at <https://thomasweise.github.io/moptipy> and <https://thomasweise.github.io/moptipyapps>.
- NumPy** is a fundamental package for scientific computing with Python, which offers efficient array datastructures<sup>18,25,31</sup>. Learn more at <https://numpy.org><sup>44</sup>.



# Glossary III

- OR** Operations Research (or Operational Research) is the application of sciences such as mathematics and computer science to the management and organization of systems, organizations, enterprises, factories, or projects. It encompasses the development and application of problem-solving methods and techniques (such as mathematical optimization, simulation, queueing theory and other stochastic models) with the goal to improve decision-making and efficiency<sup>17</sup>.
- OS** Operating System, the system that runs your computer, see, e.g., Linux, Microsoft Windows, macOS, and Android.
- PCG** A Permuted Congruential Generator (PCG) is a pseudo-random number generator<sup>46</sup>. Under NumPy, a 64-bit PCG is offered as a default method for generating seeding random number sequences<sup>45</sup>. You can import it via  
`from numpy.random import PCG64, Generator` and then create it from an `int` seed `h` via `Generator(PCG64(h))`.
- Python** The Python programming language<sup>29,37,42,66</sup>, i.e., what you will learn about in our book<sup>66</sup>. Learn more at <https://python.org>.
- QAP** The *Quadratic Assignment Problem* is an optimization problem where the goal is to assign a set of  $n$  facilities to a set of  $n$  locations<sup>8,11,34,41</sup>. Such an assignment can be represented as a permutation  $x$  of the first  $n$  natural numbers, where  $x_i$  specifies the location where facility  $i$  should be placed. For each QAP, a distance matrix  $D$  is given, where  $D_{pq}$  specifies the distance from location  $p$  to location  $q$ , as well as a flow matrix  $F$ , where  $F_{ij}$  is the amount of material flowing from facility  $i$  to facility  $j$ . The objective function  $f$  then rates a permutation  $x$  as  $f(x) = \sum_{i=1}^n \sum_{j=1}^n D_{x_i x_j} F_{ij}$ . The QAP is  $\mathcal{NP}$ -complete<sup>50</sup>.
- RLS** Randomized local search retains the best solution  $x_c$  discovered so far during the search and, in each step, it applies a unary search operator to this best-so-far solution  $x_c$  and derives a new solution  $x_n$ . If the new solution  $x_n$  is *better or equally good* when compared with  $x_c$ , i.e., not worse, then it replaces it, i.e., is stored as the new  $x_c$ . If the search space are bit strings of length  $n$ , then RLS uses a unary search operator that flips exactly one bit. This operator is the main difference to  $(1 + 1)$  evolutionary algorithm  $((1 + 1)$  EA).

# Glossary IV



- SHA-512** SHA-512 is a cryptographic hash function belonging to the *Secure Hash Algorithm 2* family<sup>51</sup>. It is a one-way function that computes a checksum of 512 bits from data of arbitrary length. For the same data, the same checksum is computed. From the checksum, you cannot obtain the original data. Under Python, you can use `from hashlib import sha512` to get such a digest from a text string `s` via `bytarray(sha512(s.encode("utf8")).digest())`. Since the digest works with binary data, we first need to convert the text to such data. Here, we did this by encoding the string to UCS Transformation Format 8 (UCS).
- stack trace** A stack trace gives information the way in which one function invoked another. The term comes from the fact that the data needed to implement function calls is stored in a stack data structure<sup>32</sup>. The data for the most recently invoked function is on top, the data of the function that called is right below, the data of the function that called that one comes next, and so on. Printing a stack trace can be very helpful when trying to find out where an `Exception` occurred.
- TSP** In an instance of the *Traveling Salesperson Problem*, also known as *Traveling Salesman Problem*, a set of  $n$  cities or locations as well as the distances between them are defined<sup>1,24,36,38,67,72</sup>. The goal is to find the shortest round-trip tour that starts at one city, visits all the other cities one time each, and returns to the origin. The TSP is one of the most well-known  $\mathcal{NP}$ -hard combinatorial optimization problems<sup>24</sup>.
- TTP** The *Traveling Tournament Problem* (TTP) is the combinatorial optimization problem of both efficiently and fairly organizing a tournament of  $n$  teams that play against each other in a pairwise fashion<sup>21,73</sup>. The efficient part boils down to arranging the games such that the total travel length is short, which is somewhat similar to the classical TSP. Initially, each team is at its home location. On each day, a team needs to travel if its scheduled game is not at its present location. On the last day, each team may need to travel back home unless their last game is a home game. The total travel length sums up the lengths of all travels over all teams. The fair part is represented in several constraints, such as `doubleRoundRobin`, `compactness`, `maxStreak`, and `noRepeat`. The TTP is  $\mathcal{NP}$ -hard<sup>62</sup>.
- Ubuntu** is a variant of the open source operating system Linux<sup>12,28</sup>. We recommend that you use this operating system to follow this class, for software development, and for research. Learn more at <https://ubuntu.com>. If you are in China, you can download it from <https://mirrors.ustc.edu.cn/ubuntu-releases>.
- UCS** Universal Coded Character Set, see Unicode



# Glossary V

- Unicode** A standard for assigning characters to numbers<sup>30,57,60</sup>. The Unicode standard supports basically all characters from all languages that are currently in use, as well as many special symbols. It is the predominantly used way to represent characters in computers and is regularly updated and improved.
- UTF-8** The *UCS Transformation Format 8* is one standard for encoding Unicode characters into a binary format that can be stored in files<sup>30,75</sup>. It is the world wide web's most commonly used character encoding, where each character is represented by one to four bytes. It is backwards compatible with ASCII.
- XML** The *Extensible Markup Language* is a text-based language for storing and transporting of data<sup>7,14,33</sup>. It allows you to define elements in the form `<myElement myAttr="x">...text..</myElement>`. Different from comma-separated values (CSV), elements in XML can be hierarchically nested, like `<a><b><c>test</c></b><b>bla</b></a>`, and thus easily represent tree structures. XML is one of most-used data interchange formats. To process XML in Python, use the `defusedxml` library<sup>27</sup>, as it protects against several security issues.
- YAML** *YAML Ain't Markup Language™* is a human-friendly data serialization language for all programming languages<sup>13,19,33</sup>. It is widely used for configuration files in the DevOps environment. See <https://yaml.org> for more information.
- $\mathcal{NP}$**  is the class of computational problems that can be solved in polynomial time by a non-deterministic machine and can be verified in polynomial time by a deterministic machine (such as a normal computer)<sup>23</sup>.
- $\mathcal{NP}$ -complete** A decision problem is  $\mathcal{NP}$ -complete if it is in  $\mathcal{NP}$  and all problems in  $\mathcal{NP}$  are reducible to it in polynomial time<sup>23,48</sup>. A problem is  $\mathcal{NP}$ -complete if it is  $\mathcal{NP}$ -hard and if it is in  $\mathcal{NP}$ .
- $\mathcal{NP}$ -hard** Algorithms that guarantee to find the correct solutions of  $\mathcal{NP}$ -hard problems<sup>10,15,35</sup> need a runtime that is exponential in the problem scale in the worst case. A problem is  $\mathcal{NP}$ -hard if all problems in  $\mathcal{NP}$  are reducible to it in polynomial time<sup>23</sup>.