Sparkle User Guide

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ADA Research Group, LIACS

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1 Quick start

Note: Sparkle currently relies on Slurm³, and does not work without it.

Follow these steps:

- 1. Install Sparkle
- 2. Prepare an algorithm configuration or an algorithm selection.
- 3. Execute commands

³ https://slurm.schedmd.com/

2 Installing Sparkle

Note: The installation process use the conda command available in Anaconda⁴ or Miniconda⁵ to manage some dependencies.

2.1 Get a copy of Sparkle

To get a copy of Sparkle you can clone the repository.

If git is available on your system, this will clone the Sparkle repository and create a subdirectory named sparkle:

\$ git clone https://bitbucket.org/sparkle-ai/sparkle.git

You can also download the stable version here: https://bitbucket.org/sparkle-ai/sparkle/get/main.zip

2.2 Install dependencies

Sparkle depends on Python 3.9+, swig 3.0, gnuplot, LaTeX, and multiple Python packages. An easy way to install most of what is needed is to use the conda package manager (https://docs.conda.io/en/latest/miniconda.html).

Note: LaTeX is used to create the reports and the documentation and must be installed manually on the system. If you don't plan to use the reports or recreate the documentations, you can skip it.

You can install the base requirements with

\$ conda env create -f environment.yml

This will create an environment named sparkle that contains everything needed to run Sparkle, except LaTeX that needs to be installed manually.

To activate the environment in the current sheel, execute:

\$ conda activate sparkle

Note: You will need to reactivate the environment every time you log in, before using Sparkle.

The file environment.yml contains a tested list of Python packages with fixed versions required to execute Sparkle. We recommended using it.

The file environment-dev.txt contains unpinned packages and the dependencies are not resolved. It is used for development and may cause problems.

The two environments can be created in parallel since one is named sparkle and the other sparkle-dev. If you want to update an environment it is better to do a clean installation by removing and recreating it. For example:

⁴ https://www.anaconda.com/

⁵ https://docs.conda.io/en/latest/miniconda.html

```
$ conda deactivate
$ conda env remove -n sparkle
$ conda env create -f environment.yml
$ conda activate sparkle
```

This should be fast as both conda and pip use local cache for the packages.

3 Algorithm Configuration

Configuring an algorithm has the following minimal requirements for the algorithm (for an example of a solver directory see Section 5.2):

- A working solver executable
- An algorithm wrapper called sprakle_smac_wrapper.py
- A PCS (parameter configuration space) file
- The runsolver binary (e.g. from Examples/Resources/Solvers/PbO-CCSAT-Generic/)

Further, training and testing instance sets are needed (for an example of an instances directory see Section 5.1). For the purpose of testing whether your configuration setup works with Sparkle, it is advised to primarily use instances that are solved (relatively) quickly even with the default parameters.

3.1 Creating a wrapper for your algorithm

A template for the wrapper that connects your algorithm with Sparkle is available at Examples/Resources/Solvers/template/sparkle_smac_wrapper.py. Within this template a number of TODOs are indicated where you are likely to need to make changes for your specific algorithm. You can also compare the different example solvers to get an idea for what kind of changes are needed.

3.2 Parameter configuration space (PCS) file

The PCS (parameter configuration space) format¹ is used to pass the possible parameter ranges of an algorithm to Sparkle in a .pcs file. For an example see e.g. Examples/Resources/Solvers/PbO-CCSAT-Generic/PbO-CCSAT-params_test.pcs.

In this file you should enter all configurable parameters of your algorithm. Note that parameters such as the random seed used by the algorithm should not be configured and therefore should also not be included in the PCS file.

4 Algorithm Selection

Creating a portfolio selector requires multiple algorithms with the following minimal requirements (for an example of a solver directory see Section 5.3):

- · A working solver executable
- An algorithm wrapper called sprakle_run_default_wrapper.py

¹ See: http://aclib.net/cssc2014/pcs-format.pdf

Further, training and testing instance sets are needed (for an example of an instances directory see Section 5.1). For the purpose of testing whether your selection setup works with Sparkle, it is advised to primarily use instances that are solved (relatively) quickly.

4.1 Creating a wrapper for your algorithm

A template for the wrapper that connects your algorithm with Sparkle is available at Examples/Resources/Solvers/template/sparkle_run_default_wrapper.py. Within this template a number of TODOs are indicated where you are likely to need to make changes for your specific algorithm. You can also compare the different example solvers to get an idea for what kind of changes are needed.

4.2 Executing commands

Executing commands in Sparkle is as simple as running them in the top directory of Sparkle, for example:

```
Commands/initialise.py
```

Do note that when running on a cluster additional arguments may be needed, for instance under Slurm the above command would change to something like:

```
srun -N1 -n1 -p graceTST Commands/initialise.py
```

In the Examples/ directory a number of common command sequences are given. For instance, for configuration with specified training and testing sets see e.g. Examples/configuration.md for an example of a sequence of commands to execute. Note that some command run in the background and need time to complete before the next command is executed. To see whether a command is still running the Slurm command squeue can be used.

In the Output/ directory paths to generated scripts and logs are gathered per executed command.

5 File structure

5.1 A typical instance directory

An instance directory should look something like this:

```
Instances/
   Example_Instance_Set/
   instance_a.cnf
   instance_b.cnf
   ...
   instance_z.cnf
```

This directory simply contains a collection of instances, as example here SAT instances in the CNF format are given.

For instances consisting of multiple files one additional file should be included in the Example_Instance_Set directory, describing which files together form an instance. The format is a signle instance per line with each file separated by a space, as shown below.

```
instance_a_part_one.abc instance_a_part_two.xyz
instance_b_part_one.abc instance_b_part_two.xyz
...
instance_z_part_one.abc instance_z_part_two.xyz
```

5.2 A typical solver directory (configuration)

A solver directory should look something like this:

```
Solver/
Example_Solver/
solver
sparkle_smac_wrapper.py
parameters.pcs
runsolver
```

Here solver is a binary executable of the solver that is to be configured. The sprakle_smac_wrapper.py is a wrapper that Sparkle should call to run the solver with specific settings, and then returns a result for the configurator. In parameters.pcs the configurable parameters are described in the PCS format. Finally, runsolver is a binary executable of the runsolver tool. This allows Sparkle to make fair time measurements for all configuration experiments.

Note: Currently the runsolver binary has to be in every solver directory, it can be found in the Examples/Resources/Solvers/PbO-CCSAT-Generic/directory.

5.3 A typical solver directory (selection)

A solver directory should look something like this:

```
Solver/
Example_Solver/
solver
sparkle_run_default_wrapper.py
```

Here solver is a binary executable of a solver that is to be included in a portfolio selector. The sprakle_run_default_wrapper.py is a wrapper that Sparkle should call to run the solver on a specific instance.

6 Wrappers

6.1 sparkle_run_default_wrapper.py

The sparkle_run_default_wrapper.py has two functions that need to be implemented for each algorithm:

```
• print_command(instance_file, seed_str: str, cutoff_time_str: str)
```

• print_output(terminal_output_file: str)

print_command(...) should print a command line call that Sparkle can use to run the algorithm on a given instance file. Ideally, for reproducibility purposes, the seed provided by Sparkle should also be passed to the algorithm. If the algorithm requires this, the cutoff time can also be passed to the algorithm. However, in this case the cutoff time should be made very large. For instance by multiplying by ten with: cutoff_time_str = str(int(cutoff_time_str) * 10). This is necessary to ensure Sparkle stops the algorithm after the cutoff time, rather than the algorithm itself. By doing this it is ensured runtime measurements are always done by Sparkle, and thus consistent between algorithms that might measure time differently.

print_output(...) should process the algorithm output. If the performance measure is RUNTIME, this function only needs to output the algorithm status. For all QUALITY performance measures both the algorithm status and the solution quality have to be given. Sparkle internally measures RUNTIME, while it can be overwritten by the user if desired, for

consistent runtime measurements between solvers this is not recommended. The output should be printed and formatted as in the example below.

```
quality 8734
status SUCCESS
```

Status can hold the following values {SUCCESS, TIMEOUT, CRASHED}. If the status is not known, reporting SUCCESS will allow Sparkle to continue, but may mean that Sparkle does not know when the algorithm crashed, and continues with faulty results.

7 Commands

Currently the commands below are available in Sparkle (listed alphabetically). Every command can be called with the -help option to get a description of the required arguments and other options.

- about.py
- add_feature_extractor.py
- · add_instances.py
- add_solver.py
- · cleanup_current_sparkle_platform.py
- cleanup_temporary_files.py
- compute_features_parallel.py
- · compute_features.py
- compute_marginal_contribution.py
- configure_solver.py
- · construct_sparkle_portfolio_selector.py
- generate_report.py
- initialise.py
- · load_record.py
- remove_feature_extractor.py
- remove_instances.py
- · remove record.py
- remove_solver.py
- run_ablation.py
- run_solvers.py
- run_sparkle_portfolio_selector.py
- run_status.py
- · save_record.py
- system_status.py
- validate_configured_vs_default.py

Arguments in [square brackets] are optional, arguments without brackets are mandatory. Input in <chevrons> indicate required text input, {curly brackets} indicate a set of inputs to choose from.

7.1 add_solver.py

Add a solver to the Sparkle platform.

Arguments:

- [--run-solver-later]
- [--parallel]
- --deterministic {0, 1}
- <solver_source_directory>

7.2 configure_solver.py

Configure a solver in the Sparkle platform.

Arguments:

- --solver <solver>
- --instance-set-train <instance-set-train>
- [--instance-set-test <instance-set-test>]
- --validate
- --ablation

Note that the test instance set is only used if the --ablation or --validation flags are given.

7.3 generate_report.py

Without any arguments a report for the most recent algorithm selection or algorithm configuration procedure is generated.

Generate a configuration report

Generate a report describing the configuration results for a solver and specific instance sets in the Sparkle platform.

Arguments:

- --solver <solver>
- [--instance-set-train <instance-set-train>]
- [--instance-set-test <instance-set-test>]

Note that if a test instance set is given, the training instance set must also be given.

7.4 initialise.py

Initialise the Sparkle platform, this command does not have any arguments.

7.5 run_ablation.py

Runs parameter importance between the default and configured parameters with ablation. This command requires a finished configuration for the solver instance pair.

Arguments:

- --solver <solver>
- [--instance-set-train <instance-set-train>]
- [--instance-set-test <instance-set-test>]

Note that if no test instance set is given, the validation is performed on the training set.

7.6 validate_configured_vs_default.py

Test the performance of the configured solver and the default solver by doing validation experiments on the training and test sets.

Arguments:

- --solver <solver>
- --instance-set-train <instance-set-train>
- [--instance-set-test <instance-set-test>]

8 Sparkle settings

Most settings can be controlled through Settings/sparkle_settings.ini. Possible settings are summarised per category in Section 8.2. For any settings that are not provided the defaults will be used. Meaning, in the extreme case, that if the settings file is empty (and nothing is set through the command line) everything will run with default values.

For convenience after every command Settings/latest.ini is written with the used settings. This can, for instance, be used to provide the same settings to the next command in a chain. E.g. for validate_configured_vs_default after configure_solver. The used settings are also recorded in the relevant Output/ subdirectory. Note that when writing settings Sparkle always uses the name, and not an alias.

8.1 Example sparkle_settings.ini

This is a short example to show the format, see the settings file in Settings/sparkle_settings.ini for more.

```
[general]
performance_measure = RUNTIME
target_cutoff_time = 60

[configuration]
number_of_runs = 25
```

(continues on next page)

```
[slurm]
number_of_runs_in_parallel = 25
```

```
8.2 Names and possible values
[general]
performance_measure
     aliases: smac_run_obj
     values: {RUNTIME, QUALITY_ABSOLUTE (also: QUALITY)}
target_cutoff_time
     aliases: smac_each_run_cutoff_time, cutoff_time_each_performance_computation
     values: integer
extractor_cutoff_time
     aliases: cutoff_time_each_feature_computation
     values: integer
penalty_multiplier
     aliases: penalty_number
     values: integer
solution_verifier
     aliases: N/A
     values: {NONE, SAT}
     note: Only available for SAT solving.
[configuration]
budget_per_run
     aliases: smac_whole_time_budget
     values: integer
number_of_runs
     aliases: num_of_smac_runs
     values: integer
[smac]
target_cutoff_length
     aliases: smac_each_run_cutoff_length
     values: {max} (other values: whatever is allowed by SMAC)
[ablation]
racing
     aliases: ablation_racing
     values: boolean
```

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[slurm]

```
number_of_runs_in_parallel
```

aliases: smac_run_obj

values: integer

clis_per_node

aliases: N/A values: integer

note: Not really a Slurm option, will likely be moved to another section.

8.3 Priorities

Settings provided through different channels have different priorities as follows:

- Default Default values will be overwritten if a value is given through any other mechanism;
- File Settings form the Settings/sparkle_settings.ini overwrite default values, but are overwritten by settings given through the command line;
- Command line file -- Settings files provided through the command line, overwrite default values and other settings files.
- Command line Settings given through the command line overwrite all other settings, including settings files provided through the command line.

8.4 Slurm (focused on Grace)

Slurm settings can be specified in the Settings/sparkle_slurm_settings.txt file. Currently these settings are inserted *as is* in any srun or sbatch calls done by Sparkle. This means that any options exclusive to one or the other currently should not be used (see Section 8.4).

Tested options

Below a list of tested Slurm options for srun and sbatch is included. Most other options for these commands should also be safe to use (given they are valid), but have not been explicitly tested. Note that any options related to commands other than srun and sbatch should not be used with Sparkle, and should not be included in Settings/sparkle_slurm_settings.txt.

- --partition / -p
- --exclude
- --nodelist

Disallowed options

The options below are exclusive to sbatch and are thus disallowed:

- --array
- --clusters
- --wrap

The options below are exclusive to srun and are thus disallowed:

• --label

Nested srun calls

A number of Sparkle commands internally call the srun command, and for those commands the provided settings need to match the restrictions of your call to a Sparkle command. Take for instance the following command:

```
srun -N1 -n1 -p graceTST Commands/configure_solver.py --solver Solvers/Pb0-CCSAT-Generic_ \leadsto --instances-train Instances/PTN/
```

This call restricts itself to the graceTST partition (the graceTST partition only consists of node 22). So if the settings file contains the setting -exclude=ethnode22, all available nodes are excluded, and the command cannot execute any internal srun commands it may have.

Finally, Slurm ignores nested partition settings for srun, but not for sbatch. This means that if you specify the graceTST partition (as above) in your command, but the graceADA partition in the settings file, Slurm will still execute any nested srun commands on the graceTST partition only.

9 Required packages

9.1 Sparkle on Grace

Grace is the computing cluster of the ADA group² at LIACS, Leiden University. Since not all packages required by Sparkle are installed on the system, some have to be installed local to the user.

Making your algorithm run on Grace

Shell and Python scripts should work as is. If a compiled binary does not work, you may have to compile it on Grace and manually install packages on Grace that are needed by your algorithm.

² http://ada.liacs.nl/

General requirements

Other software used by Sparkle:

- pdflatex
- latex
- bibtex
- gnuplot
- gnuplot-x11

To manually install gnuplot see for instance the instructions on their website http://www.gnuplot.info/development/

10 Installation and compilation of examples

10.1 Solvers

CSCCSat

CSCCSat can be recompiled as follows in the Examples/Resources/Solvers/CSCCSat/ directory:

```
unzip src.zip
cd src/CSCCSat_source_codes/
make
cp CSCCSat ../../
```

MiniSAT

MiniSAT can be recompiled as follows in the Examples/Resources/Solvers/MiniSAT/ directory:

```
unzip src.zip
cd minisat-master/
make
cp build/release/bin/minisat ../
```

PbO-CCSAT

PbO-CCSAT can be recompiled as follows in the Examples/Resources/Solvers/PbO-CCSAT-Generic/directory:

```
unzip src.zip
cd PbO-CCSAT_master/PbO-CCSAT_process_oriented_version_source_code/
make
cp PbO-CCSAT ../../
```

TCA and FastCA

The TCA and FastCA solvers, require GLIBCXX_3.4.21. This library comes with GCC 5.1.0 (or greater). Following installation you may have to update environment variables such as LD_LIBRARY_PATH, LD_RUN_PATH, CPATH to point to your installation directory.

TCA can be recompiled as follows in the Examples/Resources/CCAG/Solvers/TCA/ directory:

```
unzip src.zip
cd TCA-master/
make clean
make
cp TCA ../
```

FastCA can be recompiled as follows in the Examples/Resources/CCAG/Solvers/FastCA/ directory:

```
unzip src.zip
cd fastca-master/fastCA/
make clean
make
cp FastCA ../../
```

VRP SISRs

VRP_SISRs can be recompiled as follows in the Examples/Resources/CVRP/Solvers/VRP_SISRs/ directory:

```
unzip src.zip
cd src/
make
cp VRP_SISRs ../
```