AutoML - Benefits, Reality, Future

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Machine learning

- Widespread
- Automates human work
- Supports human experts

AutoML

Automatically construct (parts of) the machine learning pipeline

Includes, e.g.

- Data processing + cleaning
- Feature construction + selection
- Model selection
- Hyperparameter optimisation

What do we mean when we say AutoML?

Most widespread AutoML tools use meta-algorithms

- Automated algorithm configuration (including HPO + NAS)
- Automated algorithm selection

Many other ideas, but so far quite rare in practice

- Automated data processing, cleaning, etc.

Automated algorithm configuration

Improve performance by finding the best settings/parameters

- Systematic search over the parameter space
- Tries out unconventional parameter combinations
- Usually finds better performing algorithms
  [Fawcett et al. 2011, KhudaBukhsh et al. 2016, Rook et al. 2022]
- Runs while you do other things

Automated algorithm selection

Improve performance by choosing the best algorithm for the job

- Predict which algorithm to use for each problem instance
- Algorithm selection usually outperforms the single best solver

Benefits of AutoML

Performance improvement over hand designed systems

Democratise ML

- Reduce workload for ML experts
- Reduce required ML expertise

Dream: Create an ML system with one press on the button

Great benefits, great adoption?

Study AutoML adoption in software engineering for ML

- Systems where ML is used in real applications

Questionnaire [Serban et al. 2020 + 2021]

- Measure adoption levels of various AutoML techniques

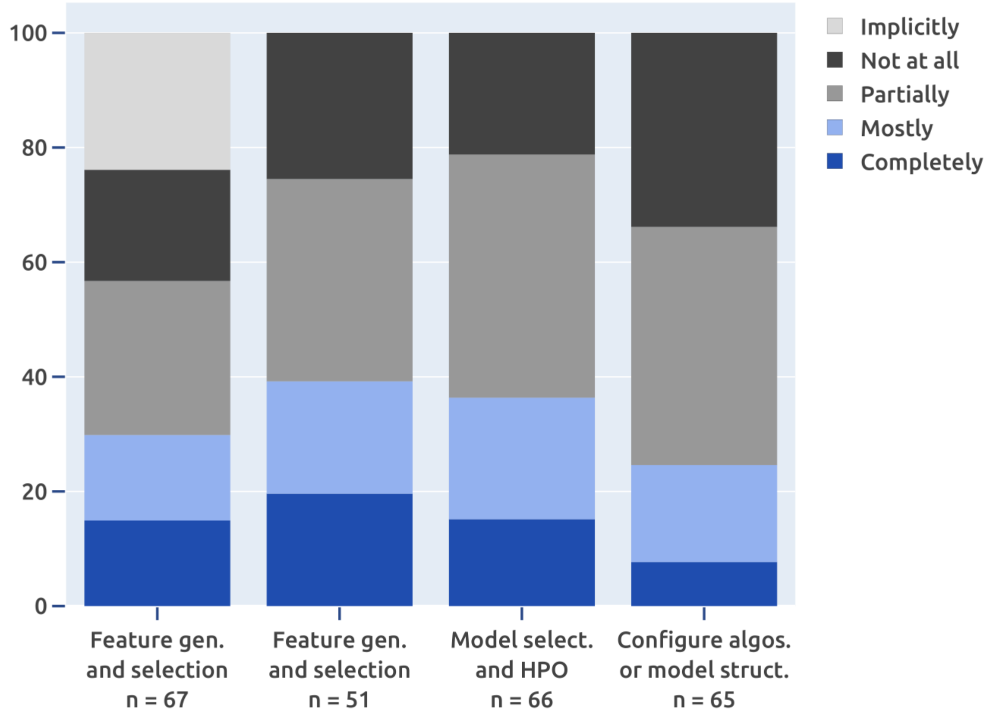
Interviews [KvdB et al. 2021]

- Insights into reasons for adoption and benefits in practice

Joint work with Alex Serban, Joost Visser & Holger Hoos

AutoML adoption is not as high as expected!

- 20-30% do not adopt AutoML at all
- Another 50-60% do not completely adopt AutoML



Why is AutoML adoption lower than expected?

Points mentioned by two interviewees

- High initial cost to adoption (missing expertise)
- Difficult to predict good run length for AutoML
- Unclear what is wrong when AutoML systems fail
- Limited availability of computational resources

Literature also suggests usability, interpretability, interactivity

What to do?

Improved AutoML systems are needed

Start with the basics

- AutoML tools for computer scientists without AutoML expertise
- Meta algorithms
  - Automated algorithm configuration
  - Automated algorithm selection

Sparkle: Accessible meta-algorithms

Lower the bar to use algorithm selection and configuration

- Ease of use: Automate where possible
- Correctness: Implement best practices, avoid pitfalls
- Explanation: Clear commands, detailed (but concise) reporting

Sparkle platform: `https://bitbucket.org/sparkle-ai/sparkle/` [KvdB et al. 2022]

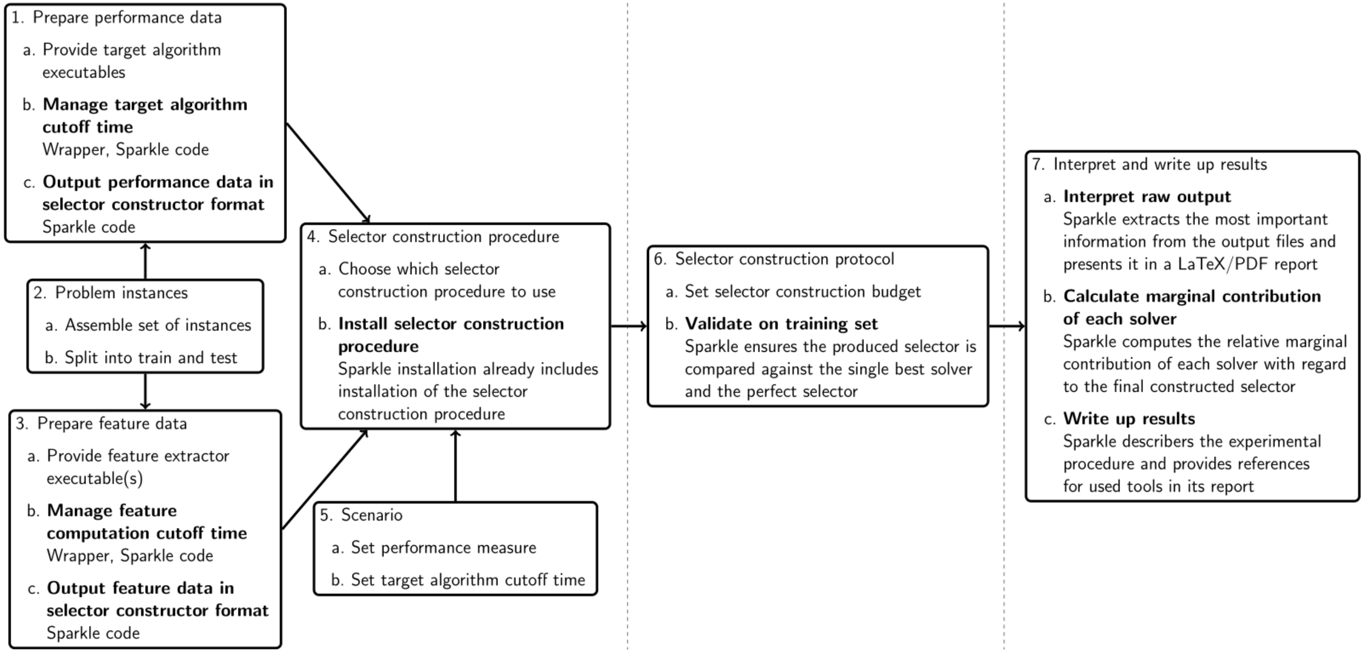
Joint work with Holger Hoos, Chuan Luo, Jeroen Rook

Algorithm selector construction

Prepare algorithm, feature extractor, wrappers, instances, selector constructor, . . .

Selector construction procedure

Result interpretation & analysis

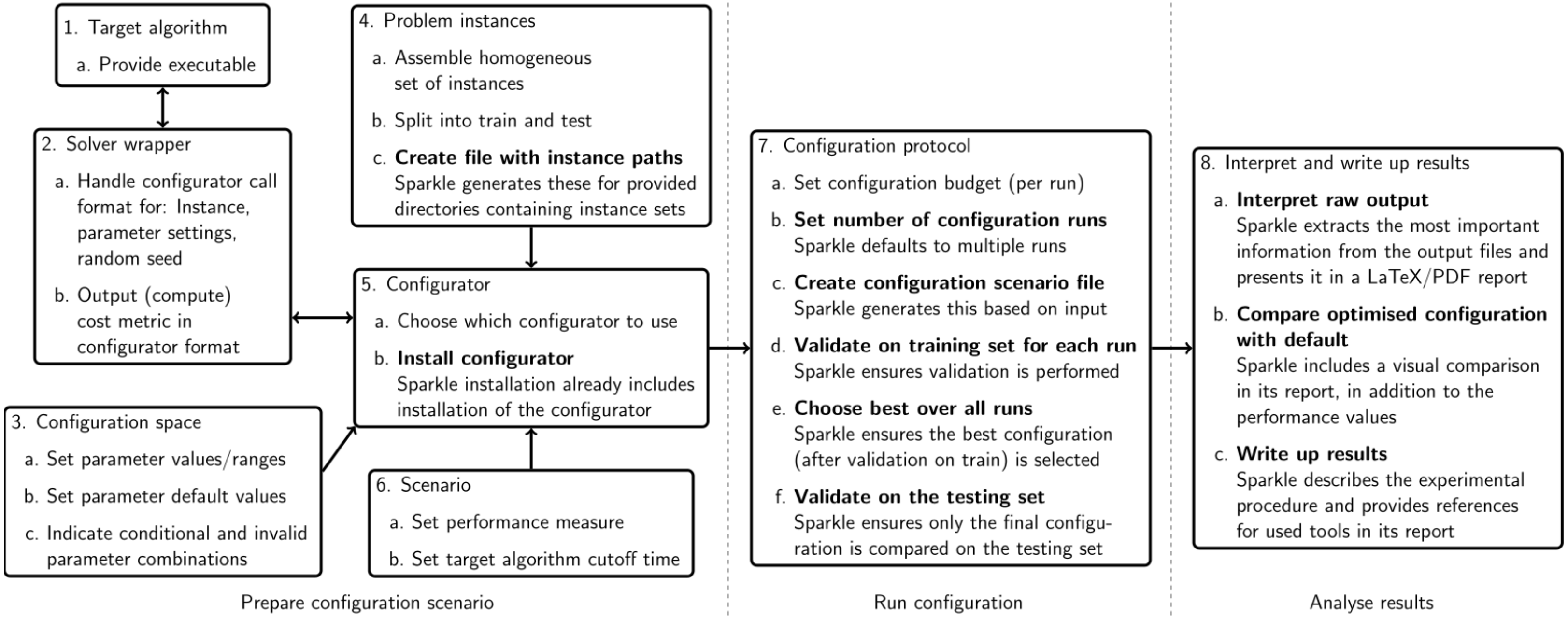


Algorithm configuration

Prepare algorithm, wrappers, parameter space, instances, configurator, . . .

Configuration procedure & execution

Result interpretation & analysis



Command example

```
1: Commands/initialise.py

2: Commands/add_instances.py Resources/PTN/

3: Commands/add_instances.py Resources/PTN2/

4: Commands/add_solver.py --deterministic 0 Resources/PbO-CSCCSAT/

5: Commands/configure_solver.py --solver PbO-CSCCSAT
--instance-set-train PTN

6: Commands/sparkle wait.py

7: Commands/validate_configured_vs_default.py
--solver Solvers/PbO-CCSAT-Generic/ --instance-set-train Instances/PTN/
--instance-set-test Instances/PTN2/

8: Commands/generate_report.py
```

Reporting

Often very basic in meta-algorithm tools (even just performance)

Detailed but concise report in Sparkle

- Used instance sets, target algorithm, configurator/selector
- Experiment description (protocol, budgets, . . .)
- Performance values + plots

Future of AutoML

No ‘one button’ magic system

Instead AutoML tools that support ML experts (eventually laymen)

- Correctness
- Understandability
- Interpretability
- Interaction

A lot of work needed beyond Sparkle!

Take away

- AutoML has the potential to democratise ML
- Only 20-30% adopt AutoML, another 50-60% only partially
- Adoption held back by missing expertise, usability, etc.
- Sparkle: Make meta-algorithms (core AutoML tools) accessible
- Future: Need tools for other audiences + AutoML components

Sparkle platform: `https://bitbucket.org/sparkle-ai/sparkle/`

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References

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