User Guide for Auto-WEKA version 2.1

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1 Introduction

Auto-WEKA is a tool that performs combined algorithm selection and hyper-parameter optimisation over the classification and regression algorithms implements in WEKA. More specifically, given a specific dataset, Auto-WEKA explores hyperparameter settings for many algorithms and recommends to a user which method will likely have good generalization performance, using model based optimisation techniques.

1.1 Availability

Auto-WEKA is available as a WEKA package through the WEKA package manager (WEKA version 3.7.13 and later). The source code is available at https://github.com/larskotthoff/autoweka, where bugs can be reported as well.

1.2 License

Auto-WEKA is open source software issued under the GNU General Public License. Note that the included SMAC optimisation method is licensed under the AGPLv3.

1.3 Requirements

Auto-WEKA does not have any additional requirements compared to WEKA. If you can run WEKA, you should be able to run Auto-WEKA.

2 User Documentation

Auto-WEKA is used much like any other WEKA classifier. After loading a dataset into WEKA, it can be run on it to automatically determine the best WEKA model and its parameters. It does so by intelligently exploring the space of classifiers and parameters using the SMAC tool (http://www.cs.ubc.ca/labs/beta/Projects/SMAC/).

A full list of all classifiers and attribute selectors along with their parameters can be found in the appendix.

2.1 Using the GUI

There are two different ways of using Auto-WEKA through the WEKA GUI. The easiest way is to use the Auto-WEKA panel, which allows you to run Auto-WEKA directly on a loaded dataset. Figure 1 shows a screenshot of a completed run.

Alternatively, Auto-WEKA can be run through the normal "Classify" panel by selecting it from the list of classifiers (Figure 2).

When using Auto-WEKA like a normal classifier, it is important to select the Test option "Use training set". Auto-WEKA performs a statistically rigorous evaluation internally and does not require an external split into training and test sets that WEKA provides. Not selecting this option will not improve the

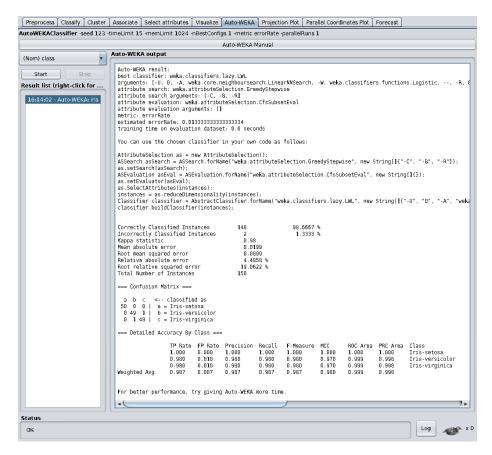


Figure 1: Auto-WEKA tab showing the output of a completed run.

quality of the result and cause Auto-WEKA to take much longer. Figure 3 shows the recommended setting.

Auto-WEKA has only a few options. Figure 4 shows them. Usually, you can leave them at their default values. For most users, only two options are relevant:

timeLimit The time in minutes Auto-WEKA will take to determine the best classifier and configuration. If you get bad results, try increasing this value.

memLimit The memory limit in Megabytes for running classifiers. If you have a very large dataset, you may need to increase this value.

While Auto-WEKA is running, it will provide the number of evaluated configurations and estimated error of the best configuration found so far in the status bar.

Note that the time limit is approximate and Auto-WEKA may not take exactly

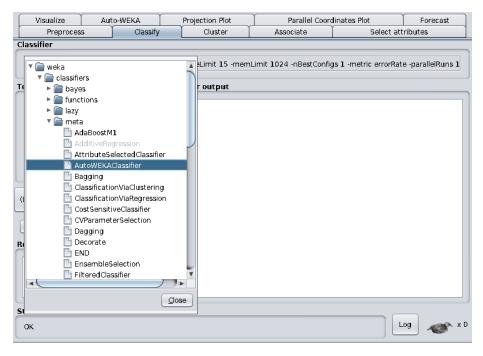


Figure 2: Location of the Auto-WEKA classifier in the list of classifiers.

as long as requested.

2.2 Running Experiments Using the CLI

Auto-WEKA can be run from the CLI like any other WEKA classifier, for example:

```
java -cp autoweka.jar weka.classifiers.meta.AutoWEKAClassifier \
    -t iris.arff -timeLimit 15 -no-cv
```

Running Auto-WEKA with the -h flag or without any options lists the options that can be set by the user:

 $\verb|java-cp| autoweka.jar| weka.classifiers.meta.AutoWEKAClassifier-h|$

Help requested.

General options:

```
-h or -help
Output help information.
-synopsis or -info
```

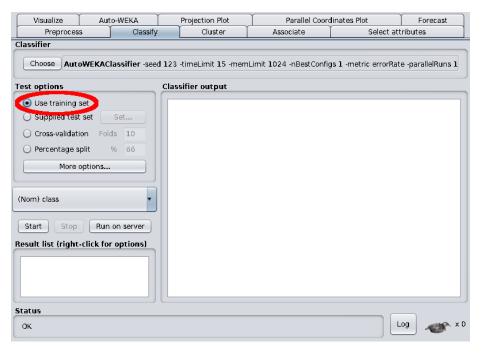


Figure 3: Recommended evaluation setting when using Auto-WEKA like a normal classifier.

```
Output synopsis for classifier (use in conjunction with -h)
-t <name of training file>
Sets training file.
-T <name of test file>
Sets test file. If missing, a cross-validation will be performed
on the training data.
-c <class index>
Sets index of class attribute (default: last).
-x <number of folds>
Sets number of folds for cross-validation (default: 10).
-no-cv
Do not perform any cross validation.
-force-batch-training
Always train classifier in batch mode, never incrementally.
-split-percentage <percentage>
Sets the percentage for the train/test set split, e.g., 66.
-preserve-order
Preserves the order in the percentage split.
-s <random number seed>
Sets random number seed for cross-validation or percentage split
```

weka.classifiers.meta.Auto	WEKAClassifier	
About		
Automatically finds th settings for a given di	e best model with its best parameter ataset.	More Capabilities
batchSize	100	
debug	False	•
doNotCheckCapabilities	False	•
memLimit	1024	
metric	errorRate	_
nBestConfigs	1	
numDecimalPlaces	2	
parallelRuns	1	
seed	123	
timeLimit	15	
Open	Save OK	Cancel

Figure 4: Auto-WEKA options.

(default: 1).

```
-m <name of file with cost matrix>
Sets file with cost matrix.
-toggle <comma-separated list of evaluation metric names>
Comma separated list of metric names to toggle in the output.
All metrics are output by default with the exception of 'Coverage' and 'Region size'.
Available metrics:
Correct,Incorrect,Kappa,Total cost,Average cost,KB relative,KB information,
Correlation,Complexity 0,Complexity scheme,Complexity improvement,
MAE,RMSE,RAE,RRSE,Coverage,Region size,TP rate,FP rate,Precision,Recall,
F-measure,MCC,ROC area,PRC area
-1 <name of input file>
```

```
Sets model input file. In case the filename ends with '.xml',
a PMML file is loaded or, if that fails, options are loaded
from the XML file.
-d <name of output file>
Sets model output file. In case the filename ends with '.xml',
only the options are saved to the XML file, not the model.
-ν
Outputs no statistics for training data.
Outputs statistics only, not the classifier.
-do-not-output-per-class-statistics
Do not output statistics for each class.
Outputs information-theoretic statistics.
-classifications "weka.classifiers.evaluation.output.prediction.AbstractOutput + options"
Uses the specified class for generating the classification output.
E.g.: weka.classifiers.evaluation.output.prediction.PlainText
Outputs predictions for test instances (or the train instances if
no test instances provided and -no-cv is used), along with the
attributes in the specified range (and nothing else).
Use '-p 0' if no attributes are desired.
Deprecated: use "-classifications ..." instead.
-distribution
Outputs the distribution instead of only the prediction
in conjunction with the '-p' option (only nominal classes).
Deprecated: use "-classifications ..." instead.
Only outputs cumulative margin distribution.
-xml filename | xml-string
Retrieves the options from the XML-data instead of the command line.
-threshold-file <file>
The file to save the threshold data to.
The format is determined by the extensions, e.g., '.arff' for ARFF
format or '.csv' for CSV.
-threshold-label <label>
The class label to determine the threshold data for
(default is the first label)
-no-predictions
Turns off the collection of predictions in order to conserve memory.
Options specific to weka.classifiers.meta.AutoWEKAClassifier:
-seed <seed>
The seed for the random number generator.
(default: 123)
```

```
-timeLimit <limit>
The time limit for tuning in minutes (approximately).
(default: 15)
-memLimit <limit>
The memory limit for runs in MiB.
(default: 1024)
-nBestConfigs <limit>
The amount of best configurations to return.
(default: 1024)
-metric <metric>
The metric to optimise.
(default: errorRate)
-parallelRuns <runs>
The number of parallel runs. EXPERIMENTAL, BE CAREFUL WHEN SETTING.
(default: 1)
-output-debug-info
If set, classifier is run in debug mode and
may output additional info to the console
-do-not-check-capabilities
If set, classifier capabilities are not checked before classifier is built
(use with caution).
-num-decimal-places
The number of decimal places for the output of numbers in the model (default 2).
-batch-size
The desired batch size for batch prediction (default 100).
```

2.3 Saving and Loading Models

Once Auto-WEKA has been run, you can save the trained model to get predictions on similar data. In the WEKA GUI, right-click on a run in the output list window and select 'Save model'. On the CLI, use the -d flag. More information on saving and loading models can be found on the WEKA wiki at https://weka.wikispaces.com/Saving+and+loading+models.

The Auto-WEKA output also contains the Java code for creating an instance of the classifier and attribute selection method that it found. This allows to retrain the model on different data.

3 Developer Documentation

Auto-WEKA's internal structure is complex and comprises more than 10,000 lines of code. A detailed explanation is beyond the scope of this document; more details can be found in the Javadoc, available at https://automl.github.io/

autoweka/. A high-level overview of the internal structure of Auto-WEKA is shown in Figure 5.

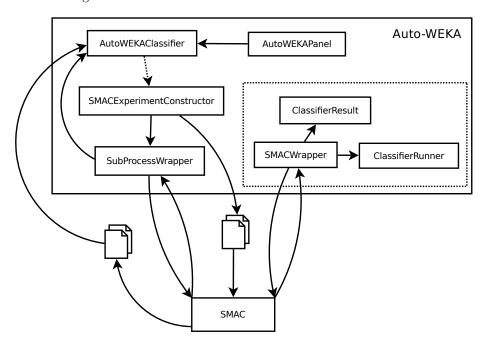


Figure 5: High-level overview of Auto-WEKA internal structure.

The user interface of Auto-WEKA is defined in the AutoWEKAClassifier and AutoWEKAPanel classes, where the latter defines the elements of the custom Auto-WEKA panel and calls AutoWEKAClassifier. New user options and additional arguments should be specified there.

The SMAC optimization tool is called through the SMACExperimentConstructor and SubProcessWrapper classes. The former prepares a set of files that contain the data, the definition of the parameter space, the training budget, and other information necessary for SMAC to run. These files are created in the system's temporary directory in a folder named autoweka<random number>. The SubProcessWrapper calls SMAC as an external process and points it to these files.

SMAC then calls Auto-WEKA's SMACWrapper class during the optimization process to evaluate the performance of a classifier and its parameters. The SMACWrapper trains and evaluates the classifier with given parameters with the ClassifierRunner class, which creates a ClassifierResult. This information is passed back to SMAC.

After SMAC's optimization completes, control is passed back to Auto-WEKA, which takes the information communicated directly from SMAC through its output and parses result files that SMAC generated. This information is used

to determine the best classifier and its parameters, which is finally presented to the user.

A Auto-WEKA Configuration Space

A.1 Classifiers, Parameters, and Parameter Ranges

Classifier	Parameter	Value Range	Default
J48	O U B J A S M	true, false true, false true, false true, false true, false true, false 1, 64 0, 1	false false false false false false 2 2 25
Decision Table	I S X	acc, rmse, mae, auc true, false BestFirst, GreedyStepwise 1, 2, 3, 4	acc false BestFirst 1
GaussianProcesses	NN E E C C C C	0001, 1 0, 1, 2 NormalizedPolyKernel, PolyKernel, Puk, RBFKernel 2, 5 true, false 2, 5 true, false 1, 10 1, 1 0001, 1	1 0 NormalizedPolyKernel 0 false 0 false 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Classifier	Parameter	Value Range	Default
M5P	N M U R.	true, false 1, 64 true, false true, false	false 4 false false false
KStar	B E M	1, 100 true, false a, d, m, n	20 false a
LMT	В С Р М W W	true, false true, false true, false true, false 1, 64 0 0, 1 true, false	false false false false 15 0 false
PART	N M R B	2, 5 1, 64 true, false true, false	3 2 false false
SMO	$_{ m M}^{ m C}$	5, 5 0, 1, 2 true, false	0 0 false

Classifier	Parameter	Value Range	Default
	Ж	NormalizedPolyKernel, PolyKernel, Puk, RBFKer-	NormalizedPolyKernel
	日	2, 5	0
	L	true, false	false
	臼	2, 5	0
	I	true, false	false
	∞	1, 10	0
	0	1, 1	0
	Ü	0001, 1	01
BayesNet	D	true, false	false
	° °	K2, HillClimber, LAGDHill-	K2
		Climber, SimulatedAnneal-	
		ing, TabuSearch, TAN	
NaiveBayes	K	true, false	false
	D	true, false	false
JRip	Z	1, 5	0
	臼	true, false	false
	Р	true, false	false
	0	1, 5	2
SimpleLogistic	S	true, false	false
	W	0	0
	W	0, 1	0

Classifier	Parameter	Value Range	Default
	A	true, false	false
LinearRegression	∞	0, 1, 2	0
	Ö	true, false	false
	$\mathbb R$	1e-7, 10	1e-7
VotedPerceptron	I	1, 10	1
1	M	5000, 50000	10000
	Э	2, 5	0
SGD	Ŧ.	0, 1, 2	0
	Т	00001, 1	01
	Я	1e-12, 10	1e-4
	Z	true, false	false
	${ m M}$	true, false	false
Logistic	R	1e-12, 10	1e-7
OneR	В	1, 32	9
MultilayerPerceptron	L	1, 1	3
	M	1, 1	2
	В	true, false	false
	H	a, i, o, t	В
	Ö	true, false	false
	R	true, false	false
	О	true, false	false
	∞	1	1

Classifier	Parameter	Value Range	Default
REPTree	M	1, 64	2
	V	1e-5, 1e-1	1e-3
	L	-1	-1
	L	2, 20	2
	P	true, false	false
IBk	E X F F	true, false 1, 64 true, false true, false true, false	false 1 false false false false
M5Rules	N U R	true, false 1, 64 true, false true, false true, false	false false false
RandomForest	I	2, 256	10
	K	0	0
	K	1, 32	2
	depth	0	0
	depth	1, 20	0
RandomTree	M	1, 64	1
	K	0	0
	K	2, 32	2
	depth	0	0

Classifier	Parameter	Value Range	Default
	depth N N U	2, 20 0 2, 5 true, false	2 0 3 false
SMOreg	NZ I E H H E L I L Z C O	5, 5 0, 1, 2 RegSMOImproved true, false NormalizedPolyKernel, PolyKernel, Puk, RBFKernel 2, 5 true, false 2, 5 true, false 1, 10 1, 10	0 BegSMOImproved false NormalizedPolyKernel false 0 false 0 false 0 false 0
Vote	G R S	0001, 1 AVG, PROD, MAJ, MIN, MAX 1	
Stacking	x x	10	10
Bagging	Ь	10, 100	100

Classifier	Parameter	Value Range	Default
	I S O	2, 128 1 true, false	10 1 false
	ч ч Г С S	100 50, 100 2, 128 true, false 1	100 100 10 false 1
	S S I	1 0, 0 2, 128	1 1 10
	K U A	-1, 10, 30, 60, 90, 120 0, 1, 2, 3, 4 LinearNNSearch	-1 0 LinearNNSearch
RandomSubSpace	I P S	2, 64 1, 0	10 1
AttributeSelectedClassifier	S E	BestFirst, GreedyStepwise CfsSubsetEval	BestFirst CfsSubsetEval
RandomCommittee	I S	2, 64	10

 ${\bf A.2}\quad {\bf Attribute\ Searches,\ Parameters,\ and\ Parameter\ Ranges}$

Attribute Search	Parameter	Value Range	Default
BestFirst	ND	0, 1, 2 $2, 10$	1 5
$\operatorname{GreedyStepwise}$	C R N	true, false true, false true, false 10, 1000	false false false 30

Default	false
Value Range	true, false true, false
Parameter	M
Attribute Evaluation	CfsSubsetEval