

CLUS: User's Manual

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Chapter 1

Introduction

This text is a user’s manual for the open source machine learning system CLUS. CLUS is a decision tree and rule learning system that works in the *predictive clustering* framework [5]. While most decision tree learners induce classification or regression trees, CLUS generalizes this approach by learning trees that are interpreted as cluster hierarchies. We call such trees predictive clustering trees or PCTs. Depending on the learning task at hand, different goal criteria are to be optimized while creating the clusters, and different heuristics will be suitable to achieve this.

Classification and regression trees are special cases of PCTs, and by choosing the right parameter settings CLUS can closely mimic the behavior of tree learners such as CART [8] or C4.5 [22]. However, its applicability goes well beyond classical classification or regression tasks: CLUS has been successfully applied to many different tasks including multi-task learning (multi-target classification and regression), structured output learning, multi-label classification, hierarchical classification, and time series prediction. Next to these supervised learning tasks, PCTs are also applicable to semi-supervised learning, subgroup discovery, and clustering. In a similar way, predictive clustering rules (PCRs) generalize classification rule sets [11] and also apply to the aforementioned learning tasks.

A full description of how CLUS works is beyond the scope of this text. In this User’s Manual, we focus on how to use CLUS: how to prepare its inputs, how to interpret the outputs, and how to change its behavior with the available parameters. This manual is a work in progress and all comments are welcome. For background information on the rationale behind the CLUS system and its algorithms we refer the reader to the following papers:

- H. Blockeel, L. De Raedt, and J. Ramon. Top-down induction of clustering trees. In *Proceedings of the 15th International Conference on Machine Learning*, pages 55–63, 1998.
- H. Blockeel and J. Struyf. Efficient algorithms for decision tree cross-validation. *Journal of Machine Learning Research*, 3: 621–650, December 2002.
- H. Blockeel, S. Džeroski, and J. Grbović. Simultaneous prediction of multiple chemical parameters of river water quality with TILDE, Proceedings of the Third European Conference on Principles of Data Mining and Knowledge Discovery (J.M. Żytkow and J. Rauch, eds.), vol 1704, LNAI, pp. 32-40, 1999.
- T. Aho, B. Ženko, and S. Džeroski. Rule ensembles for multi-target regression. In *Proceedings of 9th IEEE International Conference on Data Mining (ICDM 2009)*, pages 21–30, 2009.
- E. Fromont, H. Blockeel, and J. Struyf. Integrating decision tree learning into inductive databases. *Lecture Notes in Computer Science*, 4747: 81–96, 2007.
- D. Koccev, C. Vens, J. Struyf, and S. Džeroski. Ensembles of multi-objective decision trees. *Lecture Notes in Computer Science*, 4701: 624–631, 2007.
- I. Slavkov, V. Gjorgjioski, J. Struyf, and S. Džeroski. Finding explained groups of time-course gene expression profiles with predictive clustering trees. *Molecular Biosystems*, 2009. To appear.
- J. Struyf and S. Džeroski. Clustering trees with instance level constraints. *Lecture Notes in Computer Science*, 4701: 359–370, 2007.
- J. Struyf and S. Džeroski. Constraint based induction of multi-objective regression trees. *Lecture Notes in Computer Science*, 3933: 110–121, 2005.

- C. Vens, J. Struyf, L. Schietgat, S. Džeroski, and H. Blockeel. Decision trees for hierarchical multi-label classification. *Machine Learning*, 73 (2): 185–214, 2008.
- B. Ženko and S. Džeroski. Learning classification rules for multiple target attributes. In *Advances in Knowledge Discovery and Data Mining*, pages 454–465, 2008.

A longer list of publications describing different aspects and applications of CLUS is available on the CLUS web site (www.cs.kuleuven.be/~dtai/clus/publications.html).

Chapter 2

Getting Started

2.1 Installing and Running Clus

CLUS is written in the Java programming language, which is available from <http://java.sun.com>. You will need Java version 1.5.x or newer. To run CLUS, it suffices to install the Java Runtime Environment (JRE). If you want to make changes to CLUS and compile its source code, then you will need to install the Java Development Kit (JDK) instead of the JRE.

The CLUS software is released under the GNU General Public License version 3 or later and is available for download at <http://www.cs.kuleuven.be/~dtai/clus/>. After downloading CLUS, unpack it into a directory of your choice. CLUS is a command line application and should be started from the command prompt (Windows) or a terminal window (Unix). To start CLUS, enter the command:

```
java -jar $CLUS_DIR/Clus.jar filename.s
```

with `$CLUS_DIR/Clus.jar` the location of `Clus.jar` in your CLUS distribution and *filename.s* the name of your settings file. In order to verify that your CLUS installation is working properly, you might try something like:

Windows:

```
cd C:\Clus\data\weather
java -jar ..\..\Clus.jar weather.s
```

Unix:

```
cd $HOME/Clus/data/weather
java -jar ../../Clus.jar weather.s
```

This runs CLUS on a simple example *Weather*. You can also try other example data sets in the `data` directory of the CLUS distribution.

Note that the above instructions are for running the pre-compiled version of CLUS (`Clus.jar`), which is included with the CLUS download. If you have modified and recompiled CLUS, or if you are using the CVS version, then you should run CLUS in a different way, as is explained in Chapter 7. If you want get direct CVS access, please contact the developers.

2.2 Input and Output Files for Clus

CLUS uses (at least) two input files and these are named *filename.s* and *filename.arff*, with *filename* a name chosen by the user. The file *filename.s* contains the parameter settings for CLUS. The file *filename.arff* contains the training data to be read. The format of the data file is Weka's ARFF format¹. The results of a CLUS run are put in an output file *filename.out*. Figure 2.1 gives an overview of the input and output files supported by CLUS. The format of the data files is described in detail in Chapter 3, the format of the settings file is discussed in Chapter 4, and the output files are covered in Chapter 6. Optionally, CLUS can also generate a detailed output of the cross-validation (*weather.xval*) and model predictions in ARFF format.

¹<http://weka.wikispaces.com/ARFF>

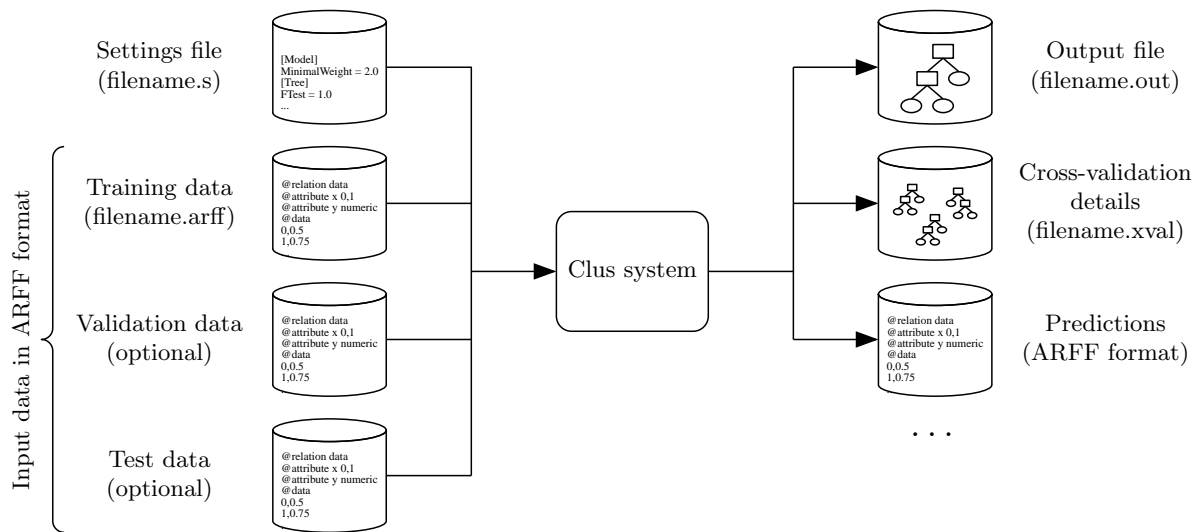


Figure 2.1: Input and output files of CLUS.

```
[Attributes]
Descriptive = 1-2
Target = 3-4
Clustering = 3-4

[Tree]
Heuristic = VarianceReduction
```

Figure 2.2: The settings file (`weather.s`) for the *Weather* example.

```
@RELATION "weather"

@ATTRIBUTE outlook      {sunny,rainy,overcast}
@ATTRIBUTE windy        {yes,no}
@ATTRIBUTE temperature  numeric
@ATTRIBUTE humidity     numeric

@DATA
sunny,    no,   34, 50
sunny,    no,   30, 55
overcast, no,   20, 70
overcast, yes,  11, 75
rainy,    no,   20, 88
rainy,    no,   18, 95
rainy,    yes,  10, 95
rainy,    yes,   8, 90
```

Figure 2.3: The training data (`weather.arff`) for the *Weather* example (in Weka's ARFF format).

2.3 A Step-by-step Example

Distribution of CLUS includes a number of example datasets. In this section we briefly take a look at the *Weather* dataset, and how it can be processed by CLUS. We use Unix notation for paths to filenames; in Windows notation the slashes become backslashes (see also previous section).

1. Move to the directory `Clus/data/weather`, which contains the *Weather* dataset:

```
cd Clus/data/weather
```

2. First inspect the file `weather.arff`. Its contents is also shown in Figure 2.3. This file contains the input data that CLUS will learn from. It is in the ARFF format: first, the name of the table is given; then, the attributes and their domains are listed; finally, the table itself is listed.
3. Next, inspect the file `weather.s`. This file is also shown in Figure 2.2. It is the *settings* file, the file where CLUS will find information about the task it should perform, values for its parameters, and other information that guides its behavior.

The *Weather* example is a small multi-target or multi-task learning problem [9], in which the goal is to predict the target attributes *temperature* and *humidity* from the input attributes *outlook* and *windy*. This kind of information is what goes in the settings file. The parameters under the heading `[Attributes]` specify the role of the different attributes. In our learning problem, the first two attributes (attributes 1-2: *outlook* and *windy*) are *descriptive* attributes: they are to be used in the cluster descriptions, that is, in the tests that appear in the predictive clustering tree's nodes (or, in rule learning, the conditions that appear in predictive clustering rules). The last two attributes (attributes 3-4) are so-called *target* attributes: these are to be predicted from the descriptive attributes. The setting `Clustering = 3-4` indicates that the clustering heuristic, which is used to construct the tree, should be computed based on the target attributes only. (That is, CLUS should try to produce clusters that are coherent with respect to the target attributes, not necessarily with respect to all attributes.) Finally, in the `Tree` section of the settings file, which contains parameters specific to tree learning, `Heuristic = VarianceReduction` specifies that, among different clustering heuristics that are available, the heuristic that should be used for this run is variance reduction.

These are only a few possible settings. Chapter 4 provides a detailed description of each setting supported by CLUS.

4. Now that we have some idea of what the settings file and data file look like, let's run CLUS on these data and see what the result is. From the Unix command line, type, in the directory where the weather files are:

```
java -jar ../../Clus.jar weather.s
```

5. CLUS now reads the data and settings files, performs its computations, and writes the resulting predictive clustering tree, together with a number of statistics such as the training set error and the test set error (if a test set has been provided), to an output file, `weather.out`. Open that file and inspect its contents; it should look like the file shown in Figure 2.4. The file contains information about the CLUS run, including some statistics, and of course also the final result: the predictive clustering tree that we wanted to learn. By default, CLUS shows both an "original model" (the tree before pruning it) and a "pruned model", which is a simplified version of the original one.

In this example, the resulting tree is a multi-target tree: each leaf predicts a vector of which the first component is the predicted *temperature* (attribute 3) and the second component the predicted *humidity* (attribute 4). A feature that distinguishes CLUS from other decision tree learners is exactly the fact that CLUS can produce this kind of trees. Constructing a multi-target tree has several advantages over constructing a separate regression tree for each target variable. The most obvious one is the number of models: the user only has to interpret one tree instead of one tree for each target. A second advantage is that the tree makes features that are relevant to all target variables explicit. For example, the first leaf of the tree in Figure 2.4 shows that `outlook = sunny` implies both a high temperature and a low humidity. Finally, due to so-called inductive transfer, multi-target PCTs may also be more accurate than regression trees. More information about multi-target trees can be found in the following publications: [5, 4, 24, 19].

```

Clus run "weather"
*****
Date: 1/10/10 12:23 PM
File: weather.out
Attributes: 4 (input: 2, output: 2)

[Data]
File = weather.arff

[Attributes]
Target = 3-4
Clustering = 3-4
Descriptive = 1-2

[Tree]
Heuristic = VarianceReduction
PruningMethod = M5

Statistics
-----
Induction Time: 0.017 sec
Pruning Time: 0.001 sec
Model information
    Original: Nodes = 7 (Leaves: 4)
    Pruned: Nodes = 3 (Leaves: 2)

Training error
-----
Number of examples: 8
Mean absolute error (MAE)
    Default      : [7.125,14.75]: 10.9375
    Original     : [2.125,2.75]: 2.4375
    Pruned       : [4.125,7.125]: 5.625
Mean squared error (MSE)
    Default      : [76.8594,275.4375]: 176.1484
    Original     : [6.5625,7.75]: 7.1562
    Pruned       : [19.4375,71.25]: 45.3438

Original Model
*****
outlook = sunny
+--yes: [32,52.5]: 2
+--no:  outlook = rainy
        +--yes: windy = yes
        |      +--yes: [9,92.5]: 2
        |      +--no:  [19,91.5]: 2
        +--no:  [15.5,72.5]: 2

Pruned Model
*****
outlook = sunny
+--yes: [32,52.5]: 2
+--no:  [14.5,85.5]: 6

```

Figure 2.4: The *Weather* example's output (`weather.out`). (Some parts have been omitted for brevity.)

Chapter 3

Input Format

Like many machine learning systems, CLUS learns from tabular data. These data are assumed to be in the ARFF format that is also used by the Weka data mining tool. Full details on ARFF can be found elsewhere¹. We here only give a minimal description.

In the data table, each row represents an instance, and each column represents an attribute of the instances. Each attribute has a name and a domain (the domain is the set of values it can take). In the ARFF format, the names and domains of the attributes are declared up front, before the data are given. The syntax is not case sensitive. An ARFF file has the following format:

```
% all comment lines are optional, start with %, and can occur
% anywhere in the file
```

```
@RELATION name
```

```
@ATTRIBUTE name domain
```

```
@ATTRIBUTE name domain
```

```
...
```

```
@DATA
```

```
value1, value2, ... , valuen
```

```
value1, value2, ... , valuen
```

The domain of an attribute can be one of:

- **numeric**
- { nomvalue₁, nomvalue₂, ... , nomvalue_n }
- **string**
- **hierarchical** hvalue₁, hvalue₂, ... , hvalue_n
- **timeseries**

The first option, **numeric** (**real** and **integer** are also legal and are treated in the same way), indicates that the domain is the set of real numbers. The second type of domain is called a discrete domain. Discrete domains are defined by enumerating the values they contain. These values are nominal. The third domain type is **string** and can be used for attributes containing arbitrary textual values.

The fourth type of domain is called **hierarchical** (multi-label). It implies two things: first, the attribute can take as a value a *set of values* from the domain, rather than just a single value; second, the domain has a hierarchical structure. The elements of the domain are typically denoted $v_1/v_2/\dots/v_i$, with $i \leq d$, where d is the depth of the hierarchy. A set of such elements is denoted by just listing them, separated by @. This type of domain is useful in the context of hierarchical multi-label classification and is not part of the standard ARFF syntax.

¹<http://weka.wikispaces.com/ARFF>

```

@RELATION HMCNewsGroups

@ATTRIBUTE word1    {1,0}
...
@ATTRIBUTE word100 {1,0}
@ATTRIBUTE class hierarchical rec/sport/swim,rec/sport/run,rec/auto,alt/atheism,...

@DATA
1,...,1,rec/sport/swim
1,...,1,rec/sport/run
1,...,1,rec/sport/run@rec/sport/swim
1,...,0,rec/sport
1,...,0,rec/auto
0,...,0,alt/atheism
...

```

Figure 3.1: An ARFF file that includes an hierarchical multi-label attribute.

```

@RELATION GeneExpressionTimeSeries

@ATTRIBUTE geneid string
@ATTRIBUTE G00000003 {1,0}
@ATTRIBUTE G00000004 {1,0}
...
@ATTRIBUTE G00051704 {1,0}
@ATTRIBUTE G00051726 {1,0}
@ATTRIBUTE target timeseries

@DATA
YAL001C,0,0,0,0,0,0,0,0,0,0,0,0,0,...,0,0,0,0,[0.07, 0.15, 0.14, 0.15,-0.11, 0.07,-0.41]
YAL002W,0,0,0,0,0,0,0,0,0,0,0,1,0,0,...,1,1,0,0,[0.14, 0.14, 0.18, 0.14, 0.17, 0.13, 0.07]
YAL003W,0,0,0,0,0,0,0,0,0,0,0,0,0,...,0,0,0,0,[0.46, 0.33, 0.04,-0.60,-0.64,-0.51,-0.36]
YAL005C,0,0,0,0,0,0,0,0,0,0,0,0,0,...,1,1,0,0,[0.86, 1.19, 1.58, 0.93, 1, 0.85, 1.24]
YAL007C,0,0,0,0,0,0,0,0,0,0,0,0,0,...,1,1,0,0,[0.12, 0.49, 0.62, 0.49, 0.84, 0.89, 1.08]
YAL008W,0,1,0,0,0,0,0,0,0,0,0,0,0,...,0,0,0,0,[0.49, 1.01, 1.33, 1.23, 1.32, 1.03, 1.14]
...

```

Figure 3.2: An ARFF file that includes an time series attribute.

The last type of domain is `timeseries`. A time series is a fixed length series of numeric data where individual numbers are written in brackets and separated with commas. All time series of a given attribute must be of the same length. This domain type, too, is not part of the standard ARFF syntax.

The values in a row occur in the same order as the attributes: the i 'th value is assigned to the i 'th attribute. The values must, obviously, be elements of the specified domain.

CLUS also supports the sparse ARFF format, where only non-zero data values are stored. The header of a sparse ARFF file is the same, but each data instance is written in curly braces and each attribute value is written as an attribute number (starting from zero) and the value separated by space; values of different attributes are separated by commas.

Figure 2.3 shows an example of an ARFF file. An example of a table containing hierarchical multi-label attributes is shown in Figure 3.1, an example ARFF file with a time series attribute is shown in Figure 3.2, and an example sparse ARFF file is shown in Figure 3.3.

```
@RELATION SparseData

@ATTRIBUTE a1      numeric
@ATTRIBUTE a2      numeric
...
@ATTRIBUTE a10     numeric
@ATTRIBUTE a11     numeric
@ATTRIBUTE class   {pos,neg}

@DATA
{1 3.1, 8 2.5, 12 pos}
{7 2.3, 12 neg}
{2 8.5, 3 1.3, 12 neg}
{1 3.2, 12 pos}
{1 3.3, 8 2.7, 12 pos}
...
```

Figure 3.3: An ARFF file in sparse format.

Chapter 4

Settings File

The algorithms included in the CLUS system have a number of parameters that influence their behavior. Most parameters have a default setting; the specification of a value for such parameters is optional. For parameters that do not have a default setting or which should get another value than the default, a value must be specified in the settings file, *filename.s*.

The settings file is structured into sections. Each parameter belongs to a particular section. Including the section headers (section names written in brackets) is optional, however; these headers are meant to help users structure the settings and their use is recommended.

We here explain the most common settings. Some settings that are connected to experimental or not yet fully implemented features of CLUS are either marked as such or not presented at all. Figure 4.1 shows an example of a settings file. All the settings (including the default ones) that were used in a specific CLUS run are printed at the beginning of the output file (*filename.out*).

In the following, we use the convention that n is an integer, r is a real, v is a vector of real values, s is a string, y is an element of { **Yes**, **No** }, r is an range of attribute indices, and o is another type of value. Strings are denoted without quotes. A vector is denoted as $[r_1, \dots, r_n]$. An attribute range is a comma separated list of integers or intervals or **None** if the range is empty. For example, 5,7-9 indicates attributes 5, 7, 8 and 9. The first attribute in the dataset is attribute 1. Run `clus -info filename.s` to list all attributes together with their indices. We now explain the settings organized into sections.

4.1 General

- **RandomSeed** = n : n is used to initialize the random generator. Some procedures used by CLUS (e.g., creation of cross-validation folds) are randomized, and as a result, different runs of CLUS on identical data may still yield different outputs. When CLUS is run on identical input data with the same **RandomSeed** setting, it is guaranteed to yield the same results.

4.2 Data

- **File** = s : s is the name of the file that contains the training set. The default value for s is *filename.arff*. CLUS can read compressed (*.arff.zip*) or uncompressed (*.arff*) data files. Path can also be included in the string.
- **TestSet** = o : when o is **None**, no test set is used; if o is a number between 0 and 1, CLUS will use a proportion o of the data file as a separate test set (used for evaluating the model but not for training); if o is a valid file name containing a test set in ARFF format, CLUS will evaluate the learned model on this test set.
- **PruneSet** = o : defines whether and how to use a pruning set; the meaning of o is identical as in the **TestSet** setting.
- **XVal** = n : n is the number of folds to be used in a cross-validation. To perform cross-validation, CLUS needs to be run with the `-xval` command line parameter.

4.3 Attributes

- **Target = r** : sets the range of target attributes. The predictive clustering model will predict these attributes. If this setting is not specified, then it is equal to the index of the last attribute in the training dataset, i.e., the last attribute is the target by default. This setting overrides the **Disable** setting. This is convenient if one needs to build models that predict only a subset S of all available target attributes T (and other target attributes should not be used as descriptive attributes). Because **Target** overrides **Disable**, one can use the settings **Disable = T** and **Target = S** to achieve this.
- **Clustering = r** : sets the range of clustering attributes. The predictive clustering heuristic that is used to guide the model construction is computed with regard to these attributes. If this setting is not specified, then the clustering attributes are by default equal to the target attributes.
- **Descriptive = r** : sets the range of attributes that can be used in the descriptive part of the models. For a PCT, these attributes will be used to construct the tests in the internal nodes of the tree. For a set of PCRs, these attributes will appear in the rule conditions. If this setting is not specified, then the descriptive attributes are all attributes that are not target, key, or disabled.
- **Disable = r** : sets the range of attributes that are to be ignored by CLUS. These attributes are also not read into memory.
- **Key = r** : sets the range of key attributes. A key attribute or a set of key attributes can be used as an example identifier. For example, if each instance represents a person, then the key attribute could store the person's name. Key attributes are not actually used by the induction algorithm, but they are written to output files, for example, to ARFF files with predictions. See **[Output]/WritePredictions** for an example.
- **Weights = o** : sets the relative weights of the different attributes in the clustering heuristic. To set the weights of all clustering attributes to 1.0, use **Weights = 1**. To use as weights $w_i = 1/\text{Var}(a_i)$, with $\text{Var}(a_i)$ the variance of attribute a_i in the input data, use **Weights = Normalize**.

4.4 Model

- **MinimalWeight = r** : CLUS only generates clusters with at least r instances in each subset (tree leaves or rules). This is a standard setting used for pre-pruning of trees and rules.

4.5 Tree

- **FTest = r** : sets the f-test stopping criterion for regression; a node will only be split if a statistical F-test indicates a significant (at level r) reduction of variance inside the subsets.
- **ConvertToRules = o** : o is an element of {**No**, **Leaves**, **AllNodes**}. CLUS can convert a tree (or ensemble of trees) into a set of rules. The default setting is **No**, if set to **Leaves**, only tree leaves are converted to rules, if set to **AllNodes**, also the internal nodes of tree(s) are converted. This setting can be used for learning rule ensembles [1].
- **Heuristic = o** : o is an element of {**Default**, **ReducedError**, **Gain**, **GainRatio**, **VarianceReduction**, **MEstimate**, **Morishita**, **DispersionAdt**, **DispersionMlt**, **RDispersionAdt**, **RDispersionMlt**}. Sets the heuristic function that is used for evaluating the clusters (splits) when generating trees or rules. Please note that this setting is used for trees as well as rules.
 - **Default**: default heuristic, if learning trees this is equal to **VarianceReduction**, if learning rules this setting is equal to **RDispersionMlt**.
 - **ReducedError**: reduced error heuristic, can be used for trees.
 - **Gain**: information gain heuristic, can be used for classification trees.
 - **GainRatio**: information gain ratio heuristic [20], can be used for classification trees.
 - **VarianceReduction**: variance reduction heuristic, can be used for trees.

- **MEstimate**: *m*-estimate heuristic [10], can be used for classification trees.
- **Morishita**: Morishita heuristic [23], can be used for trees.
- **DispersionAddt**: additive dispersion heuristic [27] pages 37–38, can be used for rules.
- **DispersionMlt**: multiplicative dispersion heuristic [27] pages 37–38, can be used for rules.
- **RDispersionAddt**: additive relative dispersion heuristic [27] pages 37–38, can be used for rules.
- **RDispersionMlt**: multiplicative relative dispersion heuristic [27] pages 37–38, can be used for rules, the default heuristic for learning predictive clustering rules.
- **PruningMethod** = *o* : *o* is an element of {**Default**, **None**, **C4.5**, **M5**, **M5Multi**, **ReducedErrorVSB**, **Garofalakis**, **GarofalakisVSB**, **CartVSB**, **CartMaxSize**}. Sets the post-pruning method for trees.
 - **Default**: default pruning method for trees, if learning classification trees this is equal to **C4.5**, if learning regression trees this is equal to **M5**.
 - **None**: no post-pruning of learned trees is performed.
 - **C4.5**: pruning as in C4.5 [22], can be used for classification trees,
 - **M5**: pruning as in M5 [21], can be used for regression trees,
 - **M5Multi**: experimental modification to M5 [21] pruning for multi-target regression trees.
 - **ReducedErrorVSB**: reduced error pruning where the error is estimated on a separate validation data set (VSB = validation set based pruning).
 - **Garofalakis**: pruning method proposed by Garofalakis et al. [13] used for constraint induction of trees.
 - **GarofalakisVSB**: same as **Garofalakis**, but the error is estimated on a separate validation data set.
 - **CartVSB**: pruning method that is implemented in CART [8], and uses a separate validation set. It seems to work better than M5 on the multi-target regression data sets.
 - **CartMaxSize**: pruning method that is also implemented in CART [8], but uses cross-validation to tune the pruning parameter to achieve the desired tree size.

4.6 Rules

- **Heuristic** = *o* : determines the heuristic for rule learning; see the Tree section for details.
- **CoveringMethod** = *o* : *o* is an element of {**Standard**, **WeightedError**, **RandomRuleSet**, **HeurOnly**, **RulesFromTree**}. Defines how the rules are generated.
 - **Standard**: standard covering algorithm [17], all examples covered by the new rule are removed from the current learning set, can be used for learning ordered rules.
 - **WeightedError**: error weighted covering algorithm [27] (Section 4.5), examples covered by the new rule are not removed from the current learning set, but their weight is decreased inversely proportional to the error the new rule makes when predicting their target values, can be used for learning unordered rules.
 - **RandomRuleSet**: rules are generated randomly, (experimental feature).
 - **HeurOnly**: no covering is used, the heuristic function takes into account the already learned rules and the examples they cover to focus on yet uncovered examples, (experimental feature).
 - **RulesFromTree**: rules are not learned with the covering approach, but a tree is learned first and then transcribed into a rule set.
- **CoveringWeight** = *r* : weight controlling the amount by which weights of covered examples are reduced within the error weighted covering algorithm – ζ in [27] (Section 4.5, Equations 4.6 and 4.8), valid values are between 0 and 1, by default it is set to 0.1, can be used for unordered rules with error weighted covering method.

- **InstCoveringWeightThreshold** = r : instance weight threshold used in error weighted covering algorithm for learning unordered rules. When an instance's weight falls below this threshold, it is removed from the current learning set. ϵ in [27] (Section 4.5), valid values are between 0 and 1, by default it is set to 0.1.
- **MaxRulesNb** = n : n defines a maximum number of rules in a rule set. By default it is set to 1000.
- **RuleAddingMethod** = o : o is an element of **{Always, IfBetter, IfBetterBeam}**. Defines how rules are added to the rule set.
 - **Always**: each rule when constructed is always added to the rule set,
 - **IfBetter**: rule is only added to the rule set if the performance of the rule set with the new rule is better than without it,
 - **IfBetterBeam**: similar to **IfBetter**, but if the rule does not improve the performance of the rule set, other rules from the beam are also evaluated and possibly added to the rule set.

The default value is **Always**, for regression rules setting this option to **IfBetter** is recommended.

- **PrintRuleWiseErrors** = y : If **Yes**, CLUS will print error estimation for each rule separately.
- **ComputedDispersion** = y : If **Yes**, CLUS will print some additional dispersion estimation for each rule and entire rule set.
- **OptGDMaxIter** = n : n defines a number of iterations that a gradient descent algorithm for optimizing rule weights makes, used for learning rule ensembles [1]. The default value is 1000.
- **OptGDMaxNbWeights** = n : n defines a maximum number of allowed nonzero weights for rules/linear terms, used for learning rule ensembles [1]. If we have enough modified weights, only the nonzero ones are altered for the rest of the optimization. With this we can limit the size of the rule set. The default value of 0 means no rule set size limitation.
- **OptGDGradTreshold** = r : the τ treshold value for the gradient descent (GD) algorithm used for learning rule ensembles [1]. τ defines the limit by which gradients are changed during every iteration of the GD algorithm. If $\tau=1$ effect is similar to L1 regularization (Lasso) and $\tau=0$ the effect is similar to L2. If **OptGDMaxNbWeights** is used, setting $\tau=1$ is usually enough (it is the fastest). Possible values are from the $[0,1]$ interval, the default is 1.
- **OptGDNbOfTParameterTry** = n : n defines how many different τ values are checked between **OptGDGradTreshold** and 1. We use a validation set to compute, which τ value gives the best accuracy. If **OptGDMaxNbWeights** is used, usually only a single value $\tau=1$ is enough (fastest).
- **OptAddLinearTerms** = o : o is an element of **{No, Yes, YesSaveMemory}**. Defines whether to add descriptive attributes as linear terms to the rule set. For some data sets, this increases the accuracy. Especially for multi-target data sets it also slows the algorithm down. For these, use value **YesSaveMemory**, otherwise it can take a lot of memory. For single target data sets **Yes** is faster. Used for learning rule ensembles [1].
- **OptLinearTermsTruncate** = y : Used in conjunction with the above **OptAddLinearTerms** setting. If **Yes**, the linear terms are truncated so that they do not predict values greater or smaller than found in the training set. This adds more resistance to outliers. The default setting is **Yes**. Used for learning rule ensembles [1].
- **OptNormalizeLinearTerms** = o : o is an element of **{No, Yes, YesAndConvert}**. Defines whether the linear terms are scaled so that each descriptive attribute has a similar effect. The default setting is **Yes** and it should always be used. However, if you want to transform the rule ensemble so that linear terms are of "standard type", you may use **YesAndConvert** setting. This moves the effect of normalizations to weights and default prediction after optimization. Used for learning rule ensembles [1].

4.7 Ensembles

- **Iterations** = n : n defines the number of base-level models (trees) in the ensemble, by default it is set to 10.
- **EnsembleMethod** = o : o is an element of `{Bagging, RForest, RSubspaces, BagSubspaces}` defines the ensemble method.
 - **Bagging**: Bagging [6].
 - **RForest**: Random forest [7].
 - **RSubspaces**: Random Subspaces [14].
 - **BagSubspaces**: Bagging of subspaces [18].
- **VotingType** = o : o is an element of `{Majority, ProbabilityDistribution}` selects the voting scheme for combining predictions of base-level models.
 - **Majority**: each base-level model casts one vote, for regression this is equal to averaging.
 - **ProbabilityDistribution**: each base-level model casts probability distributions for each target attribute, does not work for regression.

The default value is **Majority**, Bauer and Kohavi [3] recommend **ProbabilityDistribution**.

- **SelectRandomSubspaces** = n : n defines size of feature subset for random forests, random subspaces and bagging of subspaces. Default setting is 0, which means $\text{floor}(\log_2(\text{number of descriptive attributes} + 1))$ as recommended by Breiman [7].
- **PrintAllModels** = y : If **Yes**, CLUS will print all base-level models of an ensemble in the output file. The default setting is **No**.
- **PrintAllModelFiles** = y : If **Yes**, CLUS will save all base-level models of an ensemble in the model file. The default setting is **No**, which prevents from creating very large model files.
- **Optimize** = y : If **Yes**, CLUS will optimize memory usage during learning. The default setting is **No**.
- **OOBestimate** = y : If **Yes**, out-of-bag estimate of the performance of the ensemble will be done. The default setting is **No**.
- **FeatureRanking** = y : If **Yes**, feature ranking via random forests will be performed. The default setting is **No**.
- **EnsembleRandomDepth** = y : If **Yes**, different random depth for each base-level model is selected. Used, e.g., in rule ensembles. The **MaxDepth** setting from `[Tree]` section is used as average. The default setting is **No**.

4.8 Constraints

- **Syntactic** = o : sets the file with syntactic constraints (e.g., a partial tree) [24].
- **MaxSize** = o : sets the maximum size for Garofalakis pruning [13, 24]; o can be a positive integer or **Infinity**.
- **MaxError** = o : sets the maximum error for Garofalakis pruning; o is a positive real or **Infinity**.
- **MaxDepth** = o : o is a positive integer or **Infinity**. CLUS will build trees with depth at most o . In the context of rule ensemble learning [1], this sets the average maximum depth of trees that are then converted into rules and a value of 3 seems to work fine.

4.9 Output

- **AllFoldModels** = *y* : if set to **Yes**, CLUS will output the model built in each fold of a cross-validation.
- **AllFoldErrors** = *y* : if set to **Yes**, CLUS will output the test set error (and other evaluation measures) for each fold.
- **TrainErrors** = *y* : if set to **Yes**, CLUS will output the training set error (and other evaluation measures).
- **UnknownFrequency** = *y* : if set to **Yes**, CLUS will show in each node of the tree the proportion of instances that had a missing value for the test in that node.
- **BranchFrequency** = *y* : if set to **Yes**, CLUS will show in each node of the tree, for each possible outcome of the test in that node, the proportion of instances that had that outcome.
- **WritePredictions** = *o* : *o* is a subset of {**Train**, **Test**}. If *o* includes “Train”, then the prediction for each training instance will be written to an ARFF output file. The file is named *filename.train.i.pred.arff* with *i* the iteration. In a single run, *i* = 1. In a 10 fold cross-validation, *i* will vary from 1 to 10. If *o* includes “Test”, then the predictions for each test instance will be written to disk. The file is named *filename.test.pred.arff*.

4.10 Beam

- **SizePenalty** = *o* : sets the size penalty parameter used in the beam heuristic [15].
- **BeamWidth** = *n* : sets the width of the beam used in the beam search performed by CLUS [15].
- **MaxSize** = *o* : sets the maximum size constraint [15]; *o* is a positive integer or **Infinity**.

4.11 Hierarchical

A number of settings are relevant only when using CLUS for Hierarchical Multi-label Classification (HMC). These go in the separate section “Hierarchical”. The most important ones are:

- **Type** = *o* : *o* is **Tree** or **DAG**, and indicates whether the class hierarchy is a tree or a directed acyclic graph [26]
- **WType** = *o* : defines how parents’ class weights are aggregated in DAG-shaped hierarchies ([26], Section 4.1): possible values are **ExpSumParentWeight**, **ExpAvgParentWeight**, **ExpMinParentWeight**, **ExpMaxParentWeight**, and **NoWeight**. These define the weight of a class to be w_0 times the sum, average, minimum or maximum of the parent’s weights, respectively, or to be 1.0 for all classes.
- **WParam** = *r* : sets the parameter w_0 used in the formula for defining the class weights ([26], Section 4.1)
- **HSeparator** = *o* : *o* is the separator used in the notation of values of the hierarchical domain (typically ‘/’ or ‘.’)
- **EmptySetIndicator** = *o* : *o* is the symbol used to indicate the empty set
- **OptimizeErrorMeasure** = *o* : CLUS can automatically optimize the **FTest** setting; *o* indicates what criterion should be maximized for this ([26], Section 5.2). Possible values for *o* are:
 - **AverageAUROC**: average of the areas under the class-wise ROC curves
 - **AverageAUPRC**: average of the areas under the class-wise precision-recall curves
 - **WeightedAverageAUPRC**: similar to **AverageAUPRC**, but each class’s contribution is weighted by its relative frequency
 - **PooledAUPRC**: area under the average (or pooled) precision-recall curve

```

[General]
RandomSeed = 0                % seed of random generator

[Data]
File = weather.arff           % training data
TestSet = None                 % data used for evaluation (file name / proportion)
PruneSet = None                % data used for tree pruning (file name / proportion)
XVal = 10                      % number of folds in cross-validation (clus -xval ...)

[Attributes]
Target = 5                     % index of target attributes
Disable = 4                    % Disables some attributes (e.g., "5,7-8")
Key = None                     % Sets the index of the key attribute
Weights = Normalize            % Normalize numeric attributes

[Model]
MinimalWeight = 2.0            % at least 2 examples in each subtree

[Tree]
FTest = 1.0                    % f-test stopping criterion for regression
ConvertToRules = No            % Convert the tree to a set of rules

[Constraints]
Syntactic = None               % file with syntactic constraints (a partial tree)
MaxSize = Infinity             % maximum size for Garofalakis pruning
MaxError = Infinity            % maximum error for Garofalakis pruning
MaxDepth = Infinity            % Stop building the tree at the given depth

[Output]
AllFoldModels = Yes            % Output model in each cross-validation fold
AllFoldErrors = No             % Output error measures for each fold
TrainErrors = Yes              % Output training error measures
UnknownFrequency = No          % proportion of missing values for each test
BranchFrequency = No           % proportion of instances for which test succeeds
WritePredictions = {Train,Test} % write test set predictions to file

[Beam]
SizePenalty = 0.1              % size penalty parameter used in the beam heuristic
BeamWidth = 10                 % beam width
MaxSize = Infinity             % Sets the maximum size constraint

```

Figure 4.1: An example settings file

- **ClassificationThreshold = o** : The original tree constructed by CLUS contains a vector of predicted probabilities (one for each class) in each leaf. Such a probabilistic prediction can be converted into a set of labels by applying a threshold t : all labels that are predicted with probability $\geq t$ are in the predicted set. o can be a list of thresholds, e.g., [0.5, 0.75, 0.80, 0.90, 0.95]. CLUS will output for each value in the set a tree in which the predicted label sets are constructed with this particular threshold. So, in the example, the output file will contain 5 trees corresponding to the thresholds 0.5, 0.75, 0.80, 0.90 and 0.95.
- **RecallValues = v** : v is a list of recall values, e.g., [0.1, 0.2, 0.3]. For each value, CLUS will output the average of the precisions over all class-wise precision-recall curves that correspond to the particular recall value in the output file.
- **EvalClasses = o** : If o is **None**, CLUS computes average error measures across all classes in the class hierarchy. If o is a list of classes, then the error measures are only computed with regard to the classes

```

[Hierarchical]
Type = Tree                % Tree or DAG hierarchy?
WType = ExpAvgParentWeight % aggregation of class weights
WParam = 0.75              % parameter w_0
HSeparator = /             % separator used in class names
EmptySetIndicator = n      % symbol for empty set
OptimizeErrorMeasure = PooledAUPRC % FTest optimization strategy
ClassificationThreshold = None % threshold for "positive"
RecallValues = None        % where to report precision
EvalClasses = None         % classes to evaluate

```

Figure 4.2: Settings specific for hierarchical multi-label classification

in this list.

Figure 4.2 summarizes these settings briefly.

Chapter 5

Command Line Parameters

CLUS is run from the command line. It takes a number of command line parameters that affect its behavior.

- **-xval** : in addition to learning a single model from the whole input dataset, perform a cross-validation. The XVal setting (page 11) determines the number of folds; the RandomSeed setting (page 11) initializes the random generator that determines the folds.
- **-fold N** : run only fold N of the cross-validation.
- **-rules** : construct predictive clustering rules (PCRs) instead of predictive clustering trees (PCTs).
- **-forest** : construct an ensemble instead of a single tree [16].
- **-beam** : construct a tree using beam search [15].
- **-sit** : run Empirical Asymmetric Selective Transfer [19].
- **-silent** : run CLUS with reduced screen output.
- **-info** : gives information and summary statistics about the dataset.

Chapter 6

Output Files

When CLUS is finished, it writes the results of the run into an output file with the name *filename.out*. An example of such an output file is shown in Figures 6.1 to 6.4.

6.1 Used Settings

The first part of *filename.out* (shown in Figures 6.1 and 6.2) contains the values of the settings that were used for this run of CLUS, in the format used by the settings file. This part can be copied and pasted to *filename.s* and modified for subsequent runs.

6.2 Evaluation Statistics

The next part contains statistics about the results of this CLUS run.

Summary statistics about the running time of CLUS and about the size of the resulting models are given. Next, information on the models' predictive performance on the training set ("training set error") is given, as well as an estimate of its predictive performance on unseen examples ("test set error"), when available (this is the case if a cross-validation or an evaluation on a separate test set was performed).

Typically three models are reported: a "default" model consisting of a tree of size zero, which can be used as a reference point (for instance, its predictive accuracy equals that obtained by always predicting the majority class); an unpruned ("original") tree, and a pruned tree.

For classification trees the information given for each model by default includes a contingency table, and (computed from that) the accuracy and Cramer's correlation coefficient.

For regression trees, this information includes the mean absolute error (MAE), mean squared error (MSE), root mean squared error (RMSE), weighted RMSE, the Pearson correlation coefficient r and its square. In the weighted RMSE, the weight of a given attribute A is its normalization weight, which is $\frac{1}{\sqrt{\text{Var}(A)}}$, with $\text{Var}(A)$ equal to A 's variance in the input data.

6.3 The Models

The output file contains the learned models, represented as decision trees. The level of detail in which the models are shown is influenced by certain settings.

```
Clus run "weather"
*****

Date: 1/10/10 4:37 PM
File: weather.out
Attributes: 4 (input: 2, output: 2)
Missing values: No

[General]
Verbose = 1
Compatibility = Latest
RandomSeed = 0
ResourceInfoLoaded = No

[Data]
File = weather.arff
TestSet = None
PruneSet = None
XVal = 10
RemoveMissingTarget = No
NormalizeData = None

[Attributes]
Target = 3-4
Clustering = 3-4
Descriptive = 1-2
Key = None
Disable = None
Weights = Normalize
ClusteringWeights = 1.0
ReduceMemoryNominalAttrs = No

[Constraints]
Syntactic = None
MaxSize = Infinity
MaxError = 0.0
MaxDepth = Infinity

[Output]
ShowModels = {Default, Pruned, Others}
TrainErrors = Yes
ValidErrors = Yes
TestErrors = Yes
AllFoldModels = Yes
AllFoldErrors = No
AllFoldDatasets = No
UnknownFrequency = No
BranchFrequency = No
ShowInfo = {Count}
PrintModelAndExamples = No
WriteErrorFile = No
WritePredictions = {None}
WriteModelIDFiles = No
WriteCurves = No
OutputPythonModel = No
OutputDatabaseQueries = No
```

Figure 6.1: Example output file (part 1, settings).

```

[Nominal]
MEstimate = 1.0

[Model]
MinimalWeight = 2.0
MinimalNumberExamples = 0
MinimalKnownWeight = 0.0
ParamTuneNumberFolds = 10
ClassWeights = 0.0
NominalSubsetTests = Yes

[Tree]
Heuristic = VarianceReduction
PruningMethod = M5
M5PruningMult = 2.0
FTest = 1.0
BinarySplit = Yes
ConvertToRules = No
AlternativeSplits = No
Optimize = {}
MSENominal = No

```

Figure 6.2: Example output file (part 2, settings (ctd.)).

```

Run: 01
*****

Statistics
-----

FTValue (FTest): 1.0
Induction Time: 0.018 sec
Pruning Time: 0.001 sec
Model information
  Default: Nodes = 1 (Leaves: 1)
  Original: Nodes = 7 (Leaves: 4)
  Pruned: Nodes = 3 (Leaves: 2)

Training error
-----

Number of examples: 8
Mean absolute error (MAE)
  Default      : [7.125,14.75]: 10.9375
  Original     : [2.125,2.75]: 2.4375
  Pruned      : [4.125,7.125]: 5.625
Mean squared error (MSE)
  Default      : [76.8594,275.4375]: 176.1484
  Original     : [6.5625,7.75]: 7.1562
  Pruned      : [19.4375,71.25]: 45.3438
Root mean squared error (RMSE)
  Default      : [8.7669,16.5963]: 13.2721
  Original     : [2.5617,2.7839]: 2.6751
  Pruned      : [4.4088,8.441]: 6.7338
Weighted root mean squared error (RMSE) (Weights [0.013,0.004])
  Default      : [1,1]: 1
  Original     : [0.2922,0.1677]: 0.2382
  Pruned      : [0.5029,0.5086]: 0.5058
Pearson correlation coefficient
  Default      : [?,?], Avg r^2: ?
  Original     : [0.9564,0.9858], Avg r^2: 0.9432
  Pruned      : [0.8644,0.861], Avg r^2: 0.7442

```

Figure 6.3: Example output file (part 3, statistics).

```
Default Model
*****

[18.875,77.25]: 8

Original Model
*****

outlook = sunny
+--yes: [32,52.5]: 2
+--no:  outlook = rainy
        +--yes: windy = yes
        |      +--yes: [9,92.5]: 2
        |      +--no:  [19,91.5]: 2
        +--no:  [15.5,72.5]: 2

Pruned Model
*****

outlook = sunny
+--yes: [32,52.5]: 2
+--no:  [14.5,85.5]: 6
```

Figure 6.4: Example output file (part 4, learned models).

Chapter 7

Developer Documentation

7.1 Compiling Clus

Note: The CLUS download comes with a pre-compiled version of CLUS stored in the file `Clus.jar`. So, if you just want to run CLUS as it is on a data set, then you do not need to compile CLUS. You can run it by following the instructions in Section 2.1. On the other hand, if you wish to modify the source code of CLUS, or if you are using the CVS version, then you will need to compile the source code of CLUS. This can be done using the commands below or using the Eclipse IDE as pointed out in the next section.

(Windows)

```
cd C:\Clus\src
javac -d "bin" -cp ".;jars\commons-math-1.0.jar;jars\jgap.jar" clus/Clus.java
```

(Unix)

```
cd /home/john/Clus
javac -d "bin" -cp ".:jars/commons-math-1.0.jar:jars/jgap.jar" clus/Clus.java
```

This will compile CLUS and write the resulting `.class` files (Java executable byte code) to the `"bin"` subdirectory. Alternatively, use the `./compile.sh` script provided in the CLUS main directory.

7.2 Compiling Clus with Eclipse

In Eclipse, create a new project for CLUS as follows:

- Choose **File | New | Project**.
- Select "Java Project" in the dialog box.
- In the "New Java Project" dialog box:
 - Enter "Clus" in the field "Project Name".
 - Choose "Create project from existing source" and browse to the location where you unzipped Clus. E.g., `/home/john/Clus` or `C:\Clus`.
 - Click "Next".
 - Select the "Source" tab of the build settings dialog box. Change "Default output folder" (where the class files are generated) to: `"Clus/bin"`.
 - Select the "Libraries" tab of the build settings dialog box. Click "Add external jars" and add in this way these three jars:
 - `Clus/jars/commons-math-1.0.jar`
 - `Clus/jars/jgap.jar`
 - `Clus/jars/weka.jar`
 - Click "Finish".

- Select the "Navigator" view (Choose Window — Show View — Navigator)
 - Right click the "Clus" project in this view.
 - Select "Properties" from the context menu.
 - Select the "Java Compiler" tab.
 - Set the "Java Compliance Level" to 5.0.

Now CLUS should be automatically compiled by Eclipse. To run CLUS from Eclipse:

- Set as main class "clus.Clus".
- Set as arguments the name of your settings file (appfile.s).
- Set as working directory, the directory on the file system where your data set is located.

7.3 Running Clus after Compiling the Source Code

These instructions are for running CLUS after you compiled its source code (using the instructions "Compiling Clus" or "Compiling Clus with Eclipse"). To run the pre-compiled version that is available in the file "Clus.jar", see Section 2.1.

(Windows)

```
cd path\to\appfile.s
java -cp "C:\Clus\bin;C:\Clus\jars\commons-math-1.0.jar;C:\Clus\jars\jgap.jar"
clus.Clus appfile.s
```

(Unix)

```
cd path/to/appfile.s
java -cp "$HOME/Clus/bin:$HOME/Clus/jars/commons-math-1.0.jar:$HOME/Clus/jars/jgap.jar"
clus.Clus appfile.s
```

Alternatively, use the "./clus.sh" script provided in the CLUS main directory after adjusting the line that defines CLUS_DIR at the top of the script.

7.4 Code Organization

Here we only provide a rough guide to the CLUS code by listing some of the key classes and packages.

clus/Clus.java the main class with the main method, which is called when starting CLUS.

clus/algo package with learning algorithms, e.g., sub-package **clus/algo/tdidt** includes tree learning algorithm and **clus/algo/rules** includes rule learning algorithm, **clus/algo/split** includes classes used for generating conditions in both trees and rules.

clus/data package with sub-packages and classes related to reading and storing of the data.

clus/error package where different error estimation measures are defined.

clus/ext some extensions of base tree learning methods can be found here, e.g., sub-package **hierarchical** contains extensions needed for hierarchical classification, **ensembles** contains ensembles of trees and **timeseries** contains extensions for predicting time-series data.

clus/heuristic contains classes implementing heuristic functions for tree learning (heuristics for rule learning are located in package **clus/algo/rules**).

clus/main contains some important support classes such as:

```
ClusRun.java
ClusStat.java
ClusStatManager.java
```

`Settings.java` all the CLUS settings are defined here.

`clus/model` classes used for representations of models can be found here, including tests that appear in trees and rules (`clus/model/test`).

`clus/pruning` contains methods for tree pruning.

`clus/statistic` contains classes used for storing and manipulating different information and statistics on data. The key classes are:

`ClusStatistic.java` super class for all statistics used in CLUS.

`ClassificationStat.java` class for storing information on nominal attributes (e.g., counts for each possible nominal value)

`RegressionStat.java` class for storing information on numeric attributes (e.g., sums of values and sums of squared values).

`CombStat.java` class for storing information on nominal and numeric attributes (contains `ClassificationStat` and `RegressionStat` classes).

`clus/tools` contains some support code, e.g., sub-package `optimization` contains optimization procedures used in rule ensemble learning.

`clus/weka` contains classes for interfacing with Weka machine learning package.

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Appendix A

Constructing Phylogenetic Trees Using Clus

In this appendix, we describe the use of `CLUS- φ` , a method for phylogenetic tree reconstruction [25]. Example files can be found in the following directory:

`$CLUS_DIR/data/phylo/`.

The input to `CLUS- φ` consists of a multiple alignment (in ARFF format), a settings file, and optionally a distance matrix.

A.1 Input Format

Each position in the multiple alignment becomes an attribute in the ARFF file. The domain of these attributes is discrete and will typically consist of the values *A*, *C*, *T*, and *G* for DNA sequences, and the amino acids for protein sequences. If gaps occur, they have to be listed in the attribute domain. Gaps are represented as ‘-’. Moreover, `CLUS- φ` requires a string attribute, that contains an identifier for the sequence.

Perl scripts for converting PHY and FASTA files into the ARFF file format are available in the `data/phylo/` directory.

A.2 Settings File

In order to construct phylogenetic trees, the settings file looks like the one shown in Fig. A.1. Apart from the settings shown in the figure, there are a number of extra settings, specific for phylogenetic tree reconstruction (see Fig. A.2). We discuss them in detail.

- **Sequence = *o*** : defines which type of sequences is used. Possible values for *o* are **DNA**, **Protein**, or **Any**. The latter can be used in case a different alphabet than nucleotides or amino acids is used. The default value for *o* is **DNA**.
- **OptimizationCriterion = *o*** : defines which criterion is optimized in the phylogenetic tree heuristic. Possible values for *o* are **MinTotBranchLength**, for minimizing the total branch length of the tree, and **MaxAvgPWDistance**, for maximizing the average pairwise distance between two subclusters (i.e., as done in the PTDC algorithm [2]). The default value for *o* is **MinTotBranchLength**.
- **DistanceMatrix = *s*** : *s* is the name of the optional pairwise distance matrix file. This file has to be formatted in the same way as in the Phylip software package [12], i.e., the first line contains the number of sequences, and then for each sequence there is a line starting with its identifier and listing the pairwise distances to all the other sequences. See the example in the file `mydistancematrix`. The rows in the distance matrix need to have the same ordering as the rows in the ARFF file.
- **DistanceMeasure = *o*** : defines which genetic distance is used between pairs of sequences, in the case no distance matrix is given. Possible values for *o* are **Edit** for edit distance, **PDist** for p-distance, i.e., the same as edit distance, with positions with gaps or missing values discarded, **JC** for Jukes-Cantor distance, **Kimura** for Kimura distance, and **AminoKimura** for Kimura distance between amino acid sequences. See the Phylip documentation [12] for details.

```

[Tree]
PruningMethod = None
FTest = 1.0
AlternativeSplits = true      % Gives a listing of all equivalent mutations in the nodes
Heuristic = GeneticDistance

[Attributes]
Key = 1                      % The identifier attribute
Descriptive = 2-897          % All attributes corresponding to the alignment
Target = 2-897               % All attributes corresponding to the alignment
Weights = 1

[Model]
MinimalWeight = 1

[Data]
File = chimp.arff

[Output]
TrainErrors = No
PrintModelAndExamples = true

```

Figure A.1: Required settings for learning phylogenetic trees

```

[Phylogeny]
Sequence = DNA
OptimizationCriterion = MinTotBranchLength
DistanceMatrix = mydistancematrix
DistanceMeasure = JC

```

Figure A.2: Optional settings for learning phylogenetic trees

A.3 Output Files

The *filename.out* file returned by CLUS- φ can be postprocessed by the *postprocess-tree.pl* perl script in the *data/phylo/* directory. This script returns two files: *filename.clus-phy-tree*, which contains two tree representations (one with just the topology, and one with all mutations listed), and *filename.clus-phy-newick*, which contains the tree in the so-called Newick format, where clusters are represented by pairs of parentheses.

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