

Bayesian Network Classifiers in Weka for Version 3-5-7

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Abstract

Various Bayesian network classifier learning algorithms are implemented in Weka [12]. This note provides some user documentation and implementation details.

Summary of main capabilities:

- Structure learning of Bayesian networks using various hill climbing (K2, B, etc) and general purpose (simulated annealing, tabu search) algorithms.
- Local score metrics implemented; Bayes, BDe, MDL, entropy, AIC.
- \bullet Global score metrics implemented; leave one out cv, k-fold cv and cumulative cv.
- Conditional independence based causal recovery algorithm available.
- Parameter estimation using direct estimates and Bayesian model averaging.
- GUI for easy inspection and editing of Bayesian networks.
- Part of Weka allowing systematic experiments to compare Bayes net performance with general purpose classifiers like C4.5, nearest neighbor, support vector, etc.
- \bullet Source code available under GPL allows for integration in other systems and makes it easy to extend.

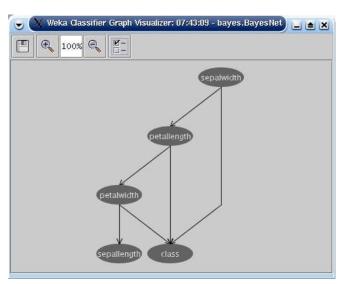
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1 Introduction

Let $U = \{x_1, \ldots, x_n\}$, $n \ge 1$ be a set of variables. A Bayesian network B over a set of variables U is a network structure B_S , which is a directed acyclic graph (DAG) over U and a set of probability tables $B_P = \{p(u|pa(u))|u \in U\}$ where pa(u) is the set of parents of u in B_S . A Bayesian network represents a probability distributions $P(U) = \prod_{u \in U} p(u|pa(u))$.

Below, a Bayesian network is shown for the variables in the iris data set. Note that the links between the nodes petallength, petalwidth and class do not form a *directed* cycle, so the graph is a proper DAG.



This picture just shows the network structure of the Bayes net, but for each of the nodes a probability distribution for the node given its parents are specified as well. For example, in the Bayes net above there is a conditional distribution for petallength given the value of sepalwidth. Since sepalwidth has no parents, there is an unconditional distribution for sepalwidth.

Basic assumptions

The classification task consist of classifying a variable $y = x_0$ called the *class variable* given a set of variables $\mathbf{x} = x_1 \dots x_n$, called *attribute variables*. A classifier $h: \mathbf{x} \to y$ is a function that maps an instance of \mathbf{x} to a value of y. The classifier is learned from a dataset D consisting of samples over (\mathbf{x}, y) . The learning task consists of finding an appropriate Bayesian network given a data set D over U.

All Bayes network algorithms implemented in Weka assume the following for the data set:

• all variables are discrete finite variables. If you have a data set with continuous variables, you can use the class weka.filters.unsupervised.attribute.Discretize to discretize them.

• no instances have missing values. If there are missing values in the data set, values are filled in using the weka.filters..unsupervised.attribute.ReplaceMissingValues filter.

The first step performed by buildClassifier is checking if the data set fulfills those assumptions. If those assumptions are not met, the data set is automatically filtered and a warning is written to STDERR.¹

Inference algorithm

To use a Bayesian network as a classifier, one simply calculates $argmax_y P(y|\mathbf{x})$ using the distribution P(U) represented by the Bayesian network. Now note that

$$P(y|\mathbf{x}) = P(U)/P(\mathbf{x})$$

$$\propto P(U)$$

$$= \prod_{u \in U} p(u|pa(u))$$
(1)

And since all variables in \mathbf{x} are known, we do not need complicated inference algorithms, but just calculate (1) for all class values.

Learning algorithms

The dual nature of a Bayesian network makes learning a Bayesian network as a two stage process a natural division: first learn a network structure, then learn the probability tables.

There are various approaches to structure learning and in Weka, the following areas are distinguished:

- local score metrics: Learning a network structure B_S can be considered an optimization problem where a quality measure of a network structure given the training data $Q(B_S|D)$ needs to be maximized. The quality measure can be based on a Bayesian approach, minimum description length, information and other criteria. Those metrics have the practical property that the score of the whole network can be decomposed as the sum (or product) of the score of the individual nodes. This allows for local scoring and thus local search methods.
- conditional independence tests: These methods mainly stem from the goal of uncovering causal structure. The assumption is that there is a network structure that exactly represents the independencies in the distribution that generated the data. Then it follows that if a (conditional) independency can be identified in the data between two variables that there is no arrow between those two variables. Once locations of edges are identified, the direction of the edges is assigned such that conditional independencies in the data are properly represented.

¹If there are missing values in the test data, but not in the training data, the values are filled in in the test data with a ReplaceMissingValues filter based on the training data.

• global score metrics: A natural way to measure how well a Bayesian network performs on a given data set is to predict its future performance by estimating expected utilities, such as classification accuracy. Cross validation provides an out of sample evaluation method to facilitate this by repeatedly splitting the data in training and validation sets. A Bayesian network structure can be evaluated by estimating the network's parameters from the training set and the resulting Bayesian network's performance determined against the validation set. The average performance of the Bayesian network over the validation sets provides a metric for the quality of the network.

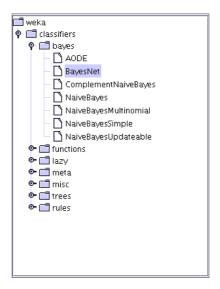
Cross validation differs from local scoring metrics in that the quality of a network structure often cannot be decomposed in the scores of the individual nodes. So, the whole network needs to be considered in order to determine the score.

• fixed structure: Finally, there are a few methods so that a structure can be fixed, for example, by reading it from an XML BIF file.

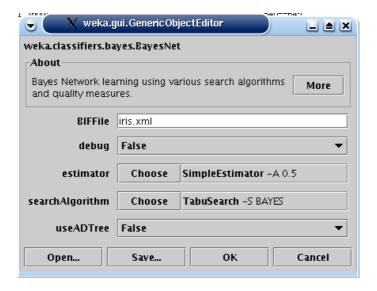
For each of these areas, different search algorithms are implemented in Weka, such as hill climbing, simulated annealing and tabu search.

Once a good network structure is identified, the conditional probability tables for each of the variables can be estimated.

You can select a Bayes net classifier by clicking the classifier 'Choose' button in the Weka explorer, experimenter or knowledge flow and find BayesNet under the weka.classifiers.bayes package (see below).



The Bayes net classifier has the following options:



The BIFFile option can be used to specify a Bayes network stored in file in BIF format [6]. When the toString method is called after learning the Bayes network, extra statistics (like extra and missing arcs) are printed comparing the network learned with the one on file.

The searchAlgorithm option can be used to select a structure learning algorithm and specify its options.

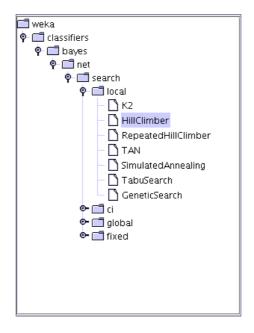
The estimator option can be used to select the method for estimating the conditional probability distributions (Section 6).

When setting the useADTree option to true, counts are calculated using the ADTree algorithm of Moore [10]. Since I have not noticed a lot of improvement for small data sets, it is set off by default. Note that this ADTree algorithm is different from the ADTree classifier algorithm from weka.classifiers.tree.ADTree.

The debug option has no effect.

2 Local score based structure learning

Distinguish score metrics (Section 2.1) and search algorithms (Section 2.2). A local score based structure learning can be selected by choosing one in the weka.classifiers.bayes.net.search.local package.



Local score based algorithms have the following options in common: initAsNaiveBayes if set true (default), the initial network structure used for starting the traversal of the search space is a naive Bayes network structure. That is, a structure with arrows from the class variable to each of the attribute variables.

If set false, an empty network structure will be used (i.e. no arrows at all). markovBlanketClassifier (False by default) if set true, at the end of the traversal of the search space, a heuristic is used to ensure each of the attributes are in the Markov blanket of the classifier node. If a node is already in the Markov blanket (ie, is a parent, child of sibling of the classifier node) nothing happens, otherwise an arrow is added.

If set **false** no such arrows are added.

scoreType determines the score metric used (See Section 2.1 for details). Currently, K2, BDe, AIC, Entropy and MDL are implemented.

maxNrOfParents is an upper bound on the number of parents of each of the nodes in the network structure learned.

2.1 Local score metrics

We use the following conventions to identify counts in the database D and a network structure B_S . Let r_i $(1 \le i \le n)$ be the cardinality of x_i . We use q_i to denote the cardinality of the parent set of x_i in B_S , that is, the number of different values to which the parents of x_i can be instantiated. So, q_i can be calculated as the product of cardinalities of nodes in $pa(x_i)$, $q_i = \prod_{x_j \in pa(x_i)} r_j$. Note $pa(x_i) = \emptyset$ implies $q_i = 1$. We use N_{ij} $(1 \le i \le n, 1 \le j \le q_i)$ to denote the number of records in D for which $pa(x_i)$ takes its jth value. We use N_{ijk} $(1 \le i \le n, 1 \le j \le q_i, 1 \le k \le r_i)$ to denote the number of records in D for which $pa(x_i)$ takes its jth value and for which x_i takes its jth value. So, $N_{ij} = \sum_{k=1}^{r_i} N_{ijk}$. We use N to denote the number of records in D.

Let the *entropy metric* $H(B_S, D)$ of a network structure and database be defined as

$$H(B_S, D) = -N \sum_{i=1}^{n} \sum_{j=1}^{q_i} \sum_{k=1}^{r_i} \frac{N_{ijk}}{N} \log \frac{N_{ijk}}{N_{ij}}$$
 (2)

and the number of parameters K as

$$K = \sum_{i=1}^{n} (r_i - 1) \cdot q_i \tag{3}$$

AIC metric The AIC metric $Q_{AIC}(B_S, D)$ of a Bayesian network structure B_S for a database D is

$$Q_{AIC}(B_S, D) = H(B_S, D) + K \tag{4}$$

A term $P(B_S)$ can be added [1] representing prior information over network structures, but will be ignored for simplicity in the Weka implementation.

MDL metric The minimum description length metric $Q_{MDL}(B_S, D)$ of a Bayesian network structure B_S for a database D is is defined as

$$Q_{MDL}(B_S, D) = H(B_S, D) + \frac{K}{2} \log N$$
(5)

Bayesian metric The Bayesian metric of a Bayesian network structure \mathcal{B}_D for a database D is

$$Q_{Bayes}(B_S, D) = P(B_S) \prod_{i=0}^{n} \prod_{j=1}^{q_i} \frac{\Gamma(N'_{ij})}{\Gamma(N'_{ij} + N_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(N'_{ijk} + N_{ijk})}{\Gamma(N'_{ijk})}$$

where $P(B_S)$ is the prior on the network structure (taken to be constant hence ignored in the Weka implementation) and $\Gamma(.)$ the gamma-function. N'_{ij} and N'_{ijk} represent choices of priors on counts restricted by $N'_{ij} = \sum_{k=1}^{r_i} N'_{ijk}$. With $N'_{ijk} = 1$ (and thus $N'_{ij} = r_i$), we obtain the K2 metric [5]

$$Q_{K2}(B_S, D) = P(B_S) \prod_{i=0}^{n} \prod_{j=1}^{q_i} \frac{(r_i - 1)!}{(r_i - 1 + N_{ij})!} \prod_{k=1}^{r_i} N_{ijk}!$$

With $N'_{ijk} = 1/(r_i \cdot q_i)$ (and thus $N'_{ij} = 1/q_i$), we obtain the **BDe metric** [8].

2.2 Search algorithms

The following search algorithms are implemented for local score metrics;

- K2 [5]: hill climbing add arcs with a fixed ordering of variables. Specific option: useRandomOrder if true a random ordering of the nodes is made at the beginning of the search. If false (default) the ordering in the data set is used. The only exception in both cases is that in case the initial network is a naive Bayes network (initAsNaiveBayes set true) the class variable is made first in the ordering.
- Hill Climbing [2]: hill climbing adding and deleting arcs with no fixed ordering of variables.

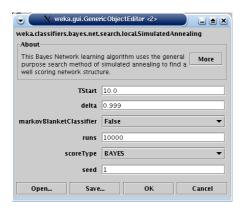
 useArcReversal if true, also arc reversals are consider when determining the next step to make.

- Repeated Hill Climber starts with a randomly generated network and then applies hill climber to reach a local optimum. The best network found is returned.
 - useArcReversal option as for Hill Climber.
- LAGD Hill Climbing does hill climbing with look ahead on a limited set of best scoring steps, implemented by Manuel. The number of look ahead steps and number of steps considered for look ahead are configurable.
- TAN [3, 7]: Tree Augmented Naive Bayes where the tree is formed by calculating the maximum weight spanning tree using Chow and Liu algorithm [4].

 No specific options.
- Simulated annealing [1]: using adding and deleting arrows. The algorithm randomly generates a candidate network B'_S close to the current network B_S . It accepts the network if it is better than the current, i.e., $Q(B'_S, D) > Q(B_S, D)$. Otherwise, it accepts the candidate with probability

 $e^{t_i \cdot (Q(B_S', D) - Q(B_S, D))}$

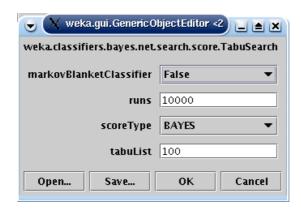
where t_i is the temperature at iteration i. The temperature starts at t_0 and is slowly decreases with each iteration.



Specific options: TStart start temperature t_0 . delta is the factor δ used to update the temperature, so $t_{i+1} = t_i \cdot \delta$. runs number of iterations used to traverse the search space. seed is the initialization value for the random number generator.

• Tabu search [1]: using adding and deleting arrows.

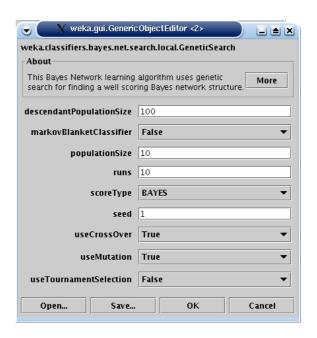
Tabu search performs hill climbing until it hits a local optimum. Then it steps to the least worse candidate in the neighborhood. However, it does not consider points in the neighborhood it just visited in the last tl steps. These steps are stored in a so called tabu-list.



Specific options: runs is the number of iterations used to traverse the search space.

tabuList is the length tl of the tabu list.

• Genetic search: applies a simple implementation of a genetic search algorithm to network structure learning. A Bayes net structure is represented by a array of $n \cdot n$ (n = number of nodes) bits where bit $i \cdot n + j$ represents whether there is an arrow from node $j \rightarrow i$.



Specific options: populationsize is the size of the population selected in each generation.

descendantPopulationsize is the number of offspring generated in each generation.

runs is the number of generation to generate.

seed is the initialization value for the random number generator.

useMutation flag to indicate whether mutation should be used. Mutation

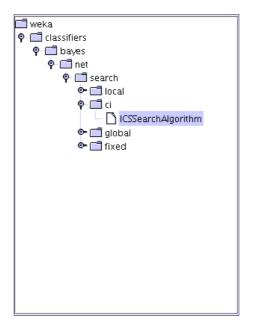
is applied by randomly adding or deleting a single arc.

useCrossOver flag to indicate whether cross-over should be used. Cross-over is applied by randomly picking an index k in the bit representation and selecting the first k bits from one and the remainder from another network structure in the population. At least one of useMutation and useCrossOver should be set to true.

useTournamentSelection when false, the best performing networks are selected from the descendant population to form the population of the next generation. When true, tournament selection is used. Tournament selection randomly chooses two individuals from the descendant population and selects the one that performs best.

3 Conditional independence test based structure learning

Conditional independence tests in Weka are slightly different from the standard tests described in the literature. To test whether variables x and y are conditionally independent given a set of variables Z, a network structure with arrows $\forall_{z \in Z} z \to y$ is compared with one with arrows $\{x \to y\} \cup \forall_{z \in Z} z \to y$. A test is performed by using any of the score metrics described in Section 2.1.



At the moment, only the ICS algorithm [11] is implemented. The algorithm makes two steps, first find a skeleton (the undirected graph with edges iff there is an arrow in network structure) and second direct all the edges in the skeleton to get a DAG.

Starting with a complete undirected graph, we try to find conditional independencies $\langle x,y|Z\rangle$ in the data. For each pair of nodes x,y, we consider sets

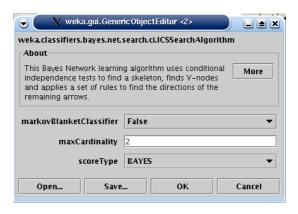
Z starting with cardinality 0, then 1 up to a user defined maximum. Furthermore, the set Z is a subset of nodes that are neighbors of both x and y. If an independency is identified, the edge between x and y is removed from the skeleton.

The first step in directing arrows is to check for every configuration x--z-y where x and y not connected in the skeleton whether z is in the set Z of variables that justified removing the link between x and y (cached in the first step). If z is not in Z, we can assign direction $x \to z \leftarrow y$.

Finally, a set of graphical rules is applied [11] to direct the remaining arrows.

Rule 5: if no edges are directed then take a random one (first we can find)

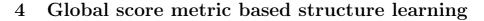
The ICS algorithm comes with the following options.

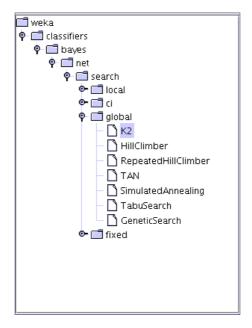


Since the ICS algorithm is focused on recovering causal structure, instead of finding the optimal classifier, the Markov blanket correction can be made afterwards.

The maxCardinality option determines the largest subset of Z to be considered in conditional independence tests $\langle x, y|Z\rangle$.

The scoreType option is used to select the scoring metric.



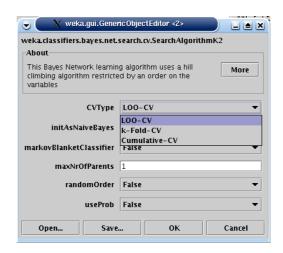


Common options for cross validation based algorithms are: initAsNaiveBayes, markovBlanketClassifier and maxNrOfParents (see Section 2 for description).

Further, for each of the cross validation based algorithms the CVType can be chosen out of the following:

- Leave one out cross validation (loo-cv) selects m = N training sets simply by taking the data set D and removing the ith record for training set D_i^t . The validation set consist of just the ith single record. Loo-cv does not always produce accurate performance estimates.
- K-fold cross validation (k-fold cv) splits the data D in m approximately equal parts D_1, \ldots, D_m . Training set D_i^t is obtained by removing part D_i from D. Typical values for m are 5, 10 and 20. With m = N, v-fold cross validation becomes loo-cv.
- Cumulative cross validation (cumulative cv) starts with an empty data set and adds instances item by item from D. After each time an item is added the next item to be added is classified using the then current state of the Bayes network.

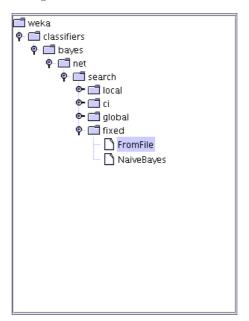
Finally, the useProb flag indicates whether the accuracy of the classifier should be estimated using the zero-one loss (if set to false) or using the estimated probability of the class.



The following search algorithms are implemented: K2, HillClimbing, RepeatedHillClimber, TAN, Tabu Search, Simulated Annealing and Genetic Search. See Section 2 for a description of the specific options for those algorithms.

5 Fixed structure 'learning'

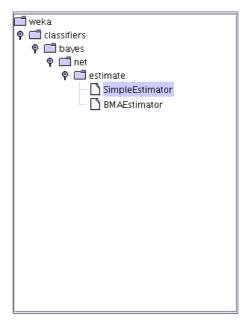
The structure learning step can be skipped by selecting a fixed network structure. There are two methods of getting a fixed structure: just make it a naive Bayes network, or reading it from a file in XML BIF format.



6 Distribution learning

Once the network structure is learned, you can choose how to learn the probability tables selecting a class in the weka.classifiers.bayes.net.estimate

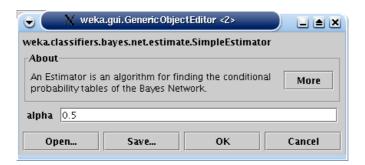
package.



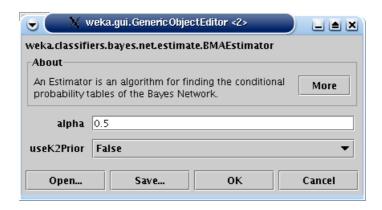
The SimpleEstimator class produces direct estimates of the conditional probabilities, that is,

$$P(x_i = k | pa(x_i) = j) = \frac{N_{ijk} + N'_{ijk}}{N_{ij} + N'_{ij}}$$

where N'_{ijk} is the alpha parameter that can be set and is 0.5 by default. With alpha=0, we get maximum likelihood estimates.



With the BMAEstimator, we get estimates for the conditional probability tables based on Bayes model averaging of all network structures that are substructures of the network structure learned [1]. This is achieved by estimating the conditional probability table of a node x_i given its parents $pa(x_i)$ as a weighted average of all conditional probability tables of x_i given subsets of $pa(x_i)$. The weight of a distribution $P(x_i|S)$ with $S \subseteq pa(x_i)$ used is proportional to the contribution of network structure $\forall_{y \in S} y \to x_i$ to either the BDe metric or K2 metric depending on the setting of the useK2Prior option (false and true respectively).



7 Running from the command line

These are the command line options of BayesNet.

```
General options:
```

```
-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).
-s <random number seed>
Sets random number seed for cross-validation (default: 1).
-m <name of file with cost matrix>
Sets file with cost matrix.
-1 <name of input file>
Sets model input file.
-d <name of output file>
Sets model output file.
Outputs no statistics for training data.
Outputs statistics only, not the classifier.
Outputs detailed information-retrieval statistics for each class.
Outputs information-theoretic statistics.
-p <attribute range>
Only outputs predictions for test instances, along with attributes (0 for none).
Only outputs cumulative margin distribution.
Only outputs the graph representation of the classifier.
Options specific to weka.classifiers.bayes.BayesNet:
```

```
-D
Do not use ADTree data structure

-B <BIF file>
BIF file to compare with

-Q weka.classifiers.bayes.net.search.SearchAlgorithm
Search algorithm

-E weka.classifiers.bayes.net.estimate.SimpleEstimator
Estimator algorithm
```

The search algorithm option -Q and estimator option -E options are mandatory.

Note that it is important that the -E options should be used after the -Q option. Extra options can be passed to the search algorithm and the estimator after the class name specified following '-'.

For example,

```
java weka.classifiers.bayes.BayesNet -t iris.arff
-Q weka.classifiers.bayes.net.search.local.SearchAlgorithmK2 -- -P
2 -S ENTROPY
-E weka.classifiers.bayes.net.estimate.SimpleEstimator -- -A 1.0
```

Overview of options for search algorithms

Options specific to weka.classifiers.bayes.net.search.local.K2:

- -N Initial structure is empty (instead of Naive Bayes)
- -P <nr of parents> Maximum number of parents
- -R Random order. (default false)
- -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.local.HillClimber:

- -P <nr of parents> Maximum number of parents
- -R Use arc reversal operation. (default false)
- -N Initial structure is empty (instead of Naive Bayes)
- -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.local.RepeatedHillClimber:

- -U <integer> Number of runs
- -A <seed> Random number seed
- -P <nr of parents> Maximum number of parents
- -R Use arc reversal operation. (default false)
- -N Initial structure is empty (instead of Naive Bayes)
- -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.local.LAGDHillClimber:

- -L <nr of look ahead steps> Number of look ahead steps
- -G <nr of good operations> Number of good operations per look ahead step.
- -P <nr of parents> Maximum number of parents
- -R Use arc reversal operation. (default false)
- -N Initial structure is empty (instead of Naive Bayes)
- -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.local.TAN:

- -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type
- Options specific to weka.classifiers.bayes.net.search.local.SimulatedAnnealing:
 - -A <float> Start temperature
 - -U <integer> Number of runs
 - -D <float> Delta temperature
 - -R < seed > Random number seed
 - -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.local.TabuSearch:

- -L <integer> Tabu list length
- -U <integer> Number of runs
- -P <nr of parents> Maximum number of parents
- -R Use arc reversal operation. (default false)
- -N Initial structure is empty (instead of Naive Bayes)
- -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.local.GeneticSearch:

- -L < integer > Population size
- -A <integer> Descendant population size
- -U <integer> Number of runs
- -M Use mutation. (default true)
- -C Use cross-over. (default true)
- -O Use tournament selection (true) or maximum subpopulation (false). (default false)
 - -R <seed> Random number seed
 - -S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.ci.ICSSearchAlgorithm:

-S [BAYES|BDeu|MDL|ENTROPY|AIC] Score type

Options specific to weka.classifiers.bayes.net.search.global.K2:

- -N Initial structure is empty (instead of Naive Bayes)
- -P <nr of parents> Maximum number of parents
- -R Random order. (default false)
- -S [LOO-CV|k-Fold-CV|Cumulative-CV] Score type
- -Q Use probabilistic or 0/1 scoring. (default probabilistic scoring)

Options specific to weka.classifiers.bayes.net.search.global.HillClimber:

- -P <nr of parents> Maximum number of parents
- -R Use arc reversal operation. (default false)
- -N Initial structure is empty (instead of Naive Bayes)
- -S [LOO-CV|k-Fold-CV|Cumulative-CV] Score type
- -Q Use probabilistic or 0/1 scoring. (default probabilistic scoring)

Options specific to weka.classifiers.bayes.net.search.global.RepeatedHillClimber:

- -U <integer> Number of runs
- -A <seed> Random number seed
- -P <nr of parents> Maximum number of parents
- -R Use arc reversal operation. (default false)
- -N Initial structure is empty (instead of Naive Bayes)
- -S [LOO-CV|k-Fold-CV|Cumulative-CV] Score type
- -Q Use probabilistic or 0/1 scoring. (default probabilistic scoring)

Options specific to weka.classifiers.bayes.net.search.global.TAN:

- -S [LOO-CV|k-Fold-CV|Cumulative-CV] Score type
- -Q Use probabilistic or 0/1 scoring. (default probabilistic scoring)

Options specific to weka.classifiers.bayes.net.search.global.SimulatedAnnealing:

- -A <float> Start temperature
- -U <integer> Number of runs
- -D <float> Delta temperature
- -R <seed> Random number seed
- -S [LOO-CV|k-Fold-CV|Cumulative-CV] Score type
- -Q Use probabilistic or 0/1 scoring. (default probabilistic scoring)

Options specific to weka.classifiers.bayes.net.search.global.TabuSearch:

- -L <integer> Tabu list length
- -U <integer> Number of runs
- -P <nr of parents> Maximum number of parents
- -R Use arc reversal operation. (default false)
- -N Initial structure is empty (instead of Naive Bayes)
- -S [LOO-CV|k-Fold-CV|Cumulative-CV] Score type
- -Q Use probabilistic or 0/1 scoring. (default probabilistic scoring)

Options specific to weka.classifiers.bayes.net.search.global.GeneticSearch:

- -L <integer> Population size
- -A <integer> Descendant population size
- -U <integer> Number of runs
- -M Use mutation. (default true)
- -C Use cross-over. (default true)
- -O Use tournament selection (true) or maximum subpopulation (false). (default false) $\,$
 - -R <seed> Random number seed
 - -S [LOO-CV|k-Fold-CV|Cumulative-CV] Score type
 - -Q Use probabilistic or 0/1 scoring. (default probabilistic scoring)

Options specific to weka.classifiers.bayes.net.search.fixed.FromFile:

-B <BIF File> Name of file containing network structure in BIF format Options specific to weka.classifiers.bayes.net.search.fixed.NaiveBayes:

Overview of options for estimators

Options specific to weka.classifiers.bayes.net.estimate.SimpleEstimator:

-A <alpha> Initial count (alpha)

Options specific to weka.classifiers.bayes.net.estimate.BMAEstimator:

-A <alpha> Initial count (alpha)

Generating random networks and artificial data sets

You can generate a random Bayes nets and data sets using weka.classifiers.bayes.net.BayesNetGenerate The options are

- -B: when specified, the network is printed, otherwise an arff file with instances randomly drawn from the network is printed.
- -N <integer>: number of nodes in the network (default 10).
- -A <integer>: number of arcs in the network (default 10).
- -C <integer>: cardinality of the variables (default 2).
- -S <integer>: random seed value (default 1).
- -M <integer>: number of instances to be generated (default 10).
- -F <filename>: read Bayes network from file instead of generating it randomly (default no file specified).

The network structure is generate by first generating a tree so that we can ensure that we have a connected graph. If any more arrows are specified they are randomly added.

8 Inspecting Bayesian networks

You can inspect some of the properties of Bayesian networks that you learned in the Explorer in text format and also in graphical format.

Bayesian networks in text

Below, you find output typical for a 10 fold cross validation run in the Weka Explorer with comments where the output is specific for Bayesian nets.

```
=== Run information ===
Scheme:
              weka.classifiers.bayes.BayesNet -S -D -B iris.xml
-Q weka.classifiers.bayes.net.search.local.TabuSearch -- -P 2
-E weka.classifiers.bayes.net.estimate.SimpleEstimator -- -A 0.5
Options for BayesNet include the class names for the structure learner and for
the distribution estimator.
Relation:
              iris-weka.filters.DiscretizeFilter-B2-Rfirst-last
Instances:
              150
Attributes:
              sepallength
              sepalwidth
              petallength
              petalwidth
              class
Test mode:
              10-fold cross-validation
=== Classifier model (full training set) ===
Bayes Network Classifier
not using ADTree
```

Indication whether the ADTree algorithm [10] for calculating counts in the data set was used.

```
#attributes=5 #classindex=4
```

This line lists the number of attribute and the number of the class variable for which the classifier was trained.

```
Network structure (nodes followed by parents) sepallength(2): petalwidth sepalwidth(2): petallength(2): sepalwidth petalwidth(2): petallength class(3): petallength petalwidth sepalwidth
```

This list specifies the network structure. Each of the variables is followed by a list of parents, so the class variable has parents petallength, petalwidth and sepalwidth while sepalwidth has no parents. The number in braces is the cardinality of the variable. It shows that in the iris dataset there are three class variables. All other variables are made binary by running it through a discretization filter.

LogScore Bayes: -479.9282866605174 LogScore BDeu: -431.83882596810105 LogScore MDL: -574.6304836846906 LogScore ENTROPY: -479.42841309686185 LogScore AIC: -517.4284130968618

These lines list the logarithmic score of the network structure for various methods of scoring.

If a BIF file was specified, the following two lines will be produced (if no such file was specified, no information is printed).

```
Missing: 1 Extra: 3 Reversed: 3 Divergence: -0.21124512294538134
```

In this case the network that was learned was compared with a file <code>iris.xml</code> which contained the naive Bayes network structure. The number after "Missing" is the number of arcs that was in the network in file that is not recovered by the structure learner. Note that a reversed arc is not counted as missing. The number after "Extra" is the number of arcs in the learned network that are not in the network on file. The number of reversed arcs is listed as well.

Finally, the divergence between the network distribution on file and the one learned is reported. This number is calculated by enumerating all possible instantiations of all variables, so it may take some time to calculate the divergence for large networks.

The remainder of the output is standard output for all classifiers.

Time taken to build model: 0.39 seconds

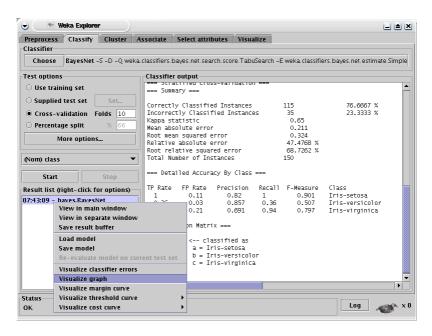
```
=== Stratified cross-validation ===
=== Summary ===
```

Correctly Classified Instances	115	76.6667 %
Incorrectly Classified Instances	35	23.3333 %

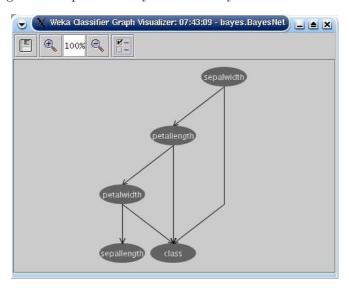
 ${
m etc...}$

Bayesian networks in GUI

To show the graphical structure, right click the appropriate BayesNet in result list of the Explorer. A menu pops up, in which you select Visualize Graph.



The Bayes network is automatically layed out and drawn thanks to a graph drawing algorithm implemented by Ashraf Kibriya.

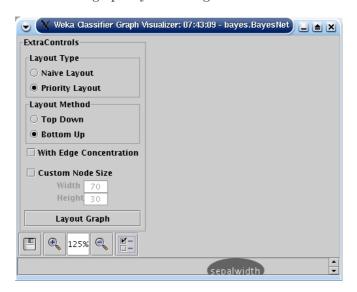


When you hover the mouse over a node, the node lights up and all its children are highlighted as well, so that it is easy to identify the relation between nodes in crowded graphs.

Saving Bayes nets You can save the Bayes network to file in the graph visualizer. You have the choice to save as XML BIF format or as dot format. Select the floppy button and a file save dialog pops up that allows you to select the file name and file format.

Zoom The graph visualizer has two buttons to zoom in and out. Also, the exact zoom desired can be entered in the zoom percentage entry. Hit enter to redraw at the desired zoom level.

Graph drawing options Hit the 'extra controls' button to show extra options that control the graph layout settings.



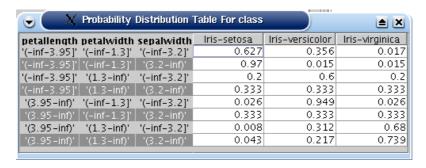
The Layout Type determines the algorithm applied to place the nodes.

The Layout Method determines in which direction nodes are considered.

The Edge Concentration toggle allows edges to be partially merged.

The Custom Node Size can be used to override the automatically determined node size.

When you click a node in the Bayesian net, a window with the probability table of the node clicked pops up. The left side shows the parent attributes and lists the values of the parents, the right side shows the probability of the node clicked conditioned on the values of the parents listed on the left.



So, the graph visualizer allows you to inspect both network structure and probability tables.

9 Bayes Network GUI

The Bayesian network editor is a stand alone application with the following features

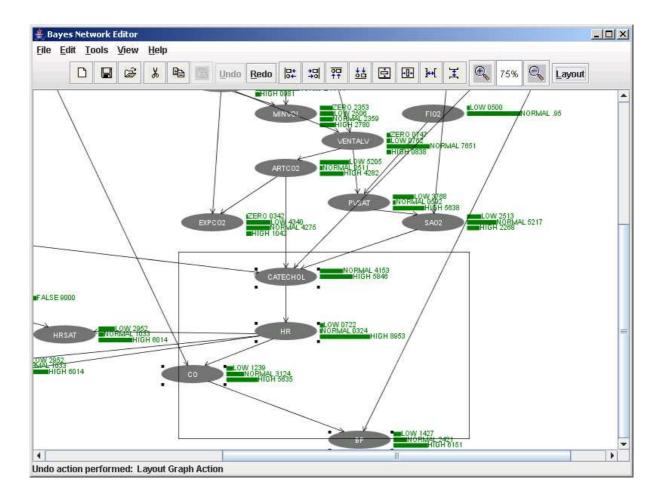
Edit Bayesian network completely by hand, with unlimited undo/redo stack,

cut/copy/paste and layout support.

- \bullet Learn Bayesian network from data using learning algorithms in Weka.
- Edit structure by hand and learn conditional probability tables (CPTs) using learning algorithms in Weka.
- Generate dataset from Bayesian network.
- Inference (using junction tree method) of evidence through the network, interactively changing values of nodes.
- Viewing cliques in junction tree.
- Accelerator key support for most common operations.

The Bayes network GUI is started as java weka.classifiers.bayes.net.GUI ibif file;

The following window pops up when an XML BIF file is specified (if none is specified an empty graph is shown).



Moving a node

Click a node with the left mouse button and drag the node to the desired position.

Selecting groups of nodes

Drag the left mouse button in the graph panel. A rectangle is shown and all nodes intersecting with the rectangle are selected when the mouse is released. Selected nodes are made visible with four little black squares at the corners (see screenshot above).

The selection can be extended by keeping the shift key pressed while selecting another set of nodes.

The selection can be toggled by keeping the ctrl key pressed. All nodes in the selection selected in the rectangle are de-selected, while the ones not in the selection but intersecting with the rectangle are added to the selection.

Groups of nodes can be moved by keeping the left mouse pressed on one of the selected nodes and dragging the group to the desired position.

File menu



The New, Save, Save As, and Exit menu provide functionality as expected. The file format used is XML BIF [6].

There are two file formats supported for opening

- .xml for XML BIF files. The Bayesian network is reconstructed from the information in the file. Node width information is not stored so the nodes are shown with the default width. This can be changed by laying out the graph (menu Tools/Layout).
- .arff Weka data files. When an arff file is selected, a new empty Bayesian network is created with nodes for each of the attributes in the arff file. Continuous variables are discretized using the weka.filters.supervised.attribute.Discretize filter (see note at end of this section for more details). The network structure can be specified and the CPTs learned using the Tools/Learn CPT menu.

The Print menu works (sometimes) as expected.

The Export menu allows for writing the graph panel to image (currently supported are bmp, jpg, png and eps formats). This can also be activated using the Alt-Shift-Left Click action in the graph panel.

Edit menu



Unlimited undo/redo support. Most edit operations on the Bayesian network are undoable. A notable exception is learning of network and CPTs.

Cut/copy/paste support. When a set of nodes is selected these can be placed on a clipboard (internal, so no interaction with other applications yet) and a paste action will add the nodes. Nodes are renamed by adding "Copy of" before the name and adding numbers if necessary to ensure uniqueness of name. Only the arrows to parents are copied, not these of the children.

The Add Node menu brings up a dialog (see below) that allows to specify the name of the new node and the cardinality of the new node. Node values are assigned the names 'Value1', 'Value2' etc. These values can be renamed (right click the node in the graph panel and select Rename Value). Another option is to copy/paste a node with values that are already properly named and rename the node.



The Add Arc menu brings up a dialog to choose a child node first;



Then a dialog is shown to select a parent. Descendants of the child node, parents of the child node and the node itself are not listed since these cannot be selected as child node since they would introduce cycles or already have an arc in the network.



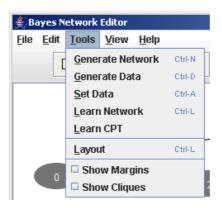
The Delete Arc menu brings up a dialog with a list of all arcs that can be deleted.



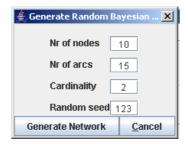
The list of eight items at the bottom are active only when a group of at least two nodes are selected.

- Align Left/Right/Top/Bottom moves the nodes in the selection such that all nodes align to the utmost left, right, top or bottom node in the selection respectively.
- Center Horizontal/Vertical moves nodes in the selection halfway between left and right most (or top and bottom most respectively).
- Space Horizontal/Vertical spaces out nodes in the selection evenly between left and right most (or top and bottom most respectively). The order in which the nodes are selected impacts the place the node is moved to.

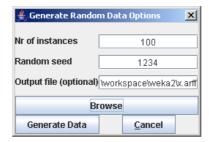
Tools menu



The Generate Network menu allows generation of a complete random Bayesian network. It brings up a dialog to specify the number of nodes, number of arcs, cardinality and a random seed to generate a network.



The Generate Data menu allows for generating a data set from the Bayesian network in the editor. A dialog is shown to specify the number of instances to be generated, a random seed and the file to save the data set into. The file format is arff. When no file is selected (field left blank) no file is written and only the internal data set is set.



The Set Data menu sets the current data set. From this data set a new Bayesian network can be learned, or the CPTs of a network can be estimated. A file choose menu pops up to select the arff file containing the data.

The Learn Network and Learn CPT menus are only active when a data set is specified either through

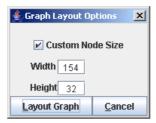
- Tools/Set Data menu, or
- Tools/Generate Data menu, or
- File/Open menu when an arff file is selected.

The Learn Network action learns the whole Bayesian network from the data set. The learning algorithms can be selected from the set available in Weka by selecting the Options button in the dialog below. Learning a network clears the undo stack.

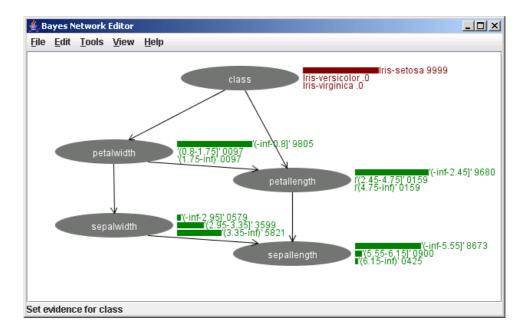


The Learn CPT menu does not change the structure of the Bayesian network, only the probability tables. Learning the CPTs clears the undo stack.

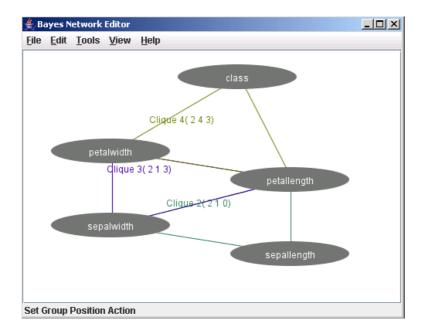
The Layout menu runs a graph layout algorithm on the network and tries to make the graph a bit more readable. When the menu item is selected, the node size can be specified or left to calculate by the algorithm based on the size of the labels by deselecting the custom node size check box.



The Show Margins menu item makes marginal distributions visible. These are calculated using the junction tree algorithm [9]. Marginal probabilities for nodes are shown in green next to the node. The value of a node can be set (right click node, set evidence, select a value) and the color is changed to red to indicate evidence is set for the node. Rounding errors may occur in the marginal probabilities.

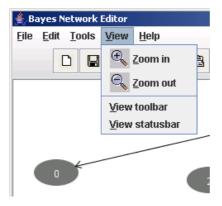


The Show Cliques menu item makes the cliques visible that are used by the junction tree algorithm. Cliques are visualized using colored undirected edges. Both margins and cliques can be shown at the same time, but that makes for rather crowded graphs.



View menu

The view menu allows for zooming in and out of the graph panel. Also, it allows for hiding or showing the status and toolbars.



Help menu

The help menu points to this document.



Toolbar



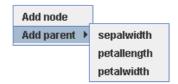
The toolbar allows a shortcut to many functions. Just hover the mouse over the toolbar buttons and a tooltiptext pops up that tells which function is activated. The toolbar can be shown or hidden with the View/View Toolbar menu.

Statusbar

At the bottom of the screen the statusbar shows messages. This can be helpful when an undo/redo action is performed that does not have any visible effects, such as edit actions on a CPT. The statusbar can be shown or hidden with the View/View Statusbar menu.

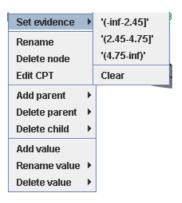
Click right mouse button

Clicking the right mouse button in the graph panel outside a node brings up the following popup menu. It allows to add a node at the location that was clicked, or add select a parent to add to all nodes in the selection. If no node is selected, or no node can be added as parent, this function is disabled.

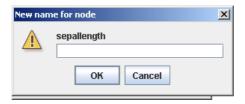


Clicking the right mouse button on a node brings up a popup menu.

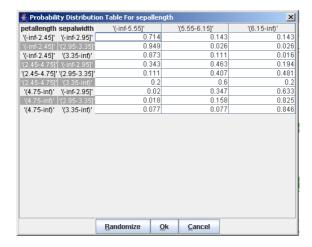
The popup menu shows list of values that can be set as evidence to selected node. This is only visible when margins are shown (menu Tools/Show margins). By selecting 'Clear', the value of the node is removed and the margins calculated based on CPTs again.



A node can be renamed by right click and select Rename in the popup menu. The following dialog appears that allows entering a new node name.

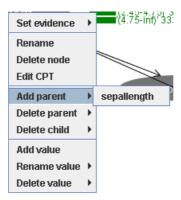


The CPT of a node can be edited manually by selecting a node, right click/Edit CPT. A dialog is shown with a table representing the CPT. When a value is edited, the values of the remainder of the table are update in order to ensure that the probabilities add up to 1. It attempts to adjust the last column first, then goes backward from there.

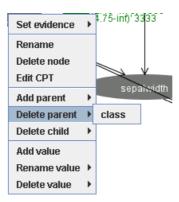


The whole table can be filled with randomly generated distributions by selecting the Randomize button.

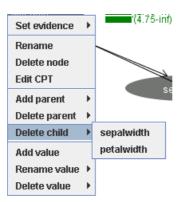
The popup menu shows list of parents that can be added to selected node. CPT for the node is updated by making copies for each value of the new parent.



The popup menu shows list of parents that can be deleted from selected node. CPT of the node keeps only the one conditioned on the first value of the parent node.



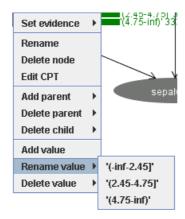
The popup menu shows list of children that can be deleted from selected node. CPT of the child node keeps only the one conditioned on the first value of the parent node.



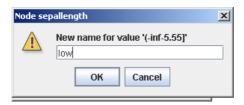
Selecting the Add Value from the popup menu brings up this dialog, in which the name of the new value for the node can be specified. The distribution for the node assign zero probability to the value. Child node CPTs are updated by copying distributions conditioned on the new value.



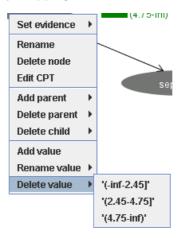
The popup menu shows list of values that can be renamed for selected node.



Selecting a value brings up the following dialog in which a new name can be specified.



The popup menu shows list of values that can be deleted from selected node. This is only active when there are more then two values for the node (single valued nodes do not make much sense). By selecting the value the CPT of the node is updated in order to ensure that the CPT adds up to unity. The CPTs of children are updated by dropping the distributions conditioned on the value.



A note on CPT learning

Continuous variables are discretized by the Bayes network class. The discretization algorithm chooses its values based on the information in the data set.

However, these values are not stored anywhere. So, reading an arff file with continuous variables using the File/Open menu allows one to specify a network, then learn the CPTs from it since the discretization bounds are still known. However, opening an arff file, specifying a structure, then closing the application, reopening and trying to learn the network from another file containing continuous variables may not give the desired result since a the discretization algorithm is re-applied and new boundaries may have been found. Unexpected behavior may be the result.

Learning from a dataset that contains more attributes than there are nodes in the network is ok. The extra attributes are just ignored.

Learning from a dataset with differently ordered attributes is ok. Attributes are matched to nodes based on name. However, attribute values are matched with node values based on the order of the values.

The attributes in the dataset should have the same number of values as the corresponding nodes in the network (see above for continuous variables).

10 Bayesian nets in the experimenter

Bayesian networks generate extra measures that can be examined in the experimenter. The experimenter can then be used to calculate mean and variance for those measures.

The following metrics are generated:

- measureExtraArcs: extra arcs compared to reference network. The network must be provided as BIFFile to the BayesNet class. If no such network is provided, this value is zero.
- measureMissingArcs: missing arcs compared to reference network or zero if not provided.
- measureReversedArcs: reversed arcs compared to reference network or zero if not provided.
- measureDivergence: divergence of network learned compared to reference network or zero if not provided.
- measureBayesScore: log of the K2 score of the network structure.
- measureBDeuScore: log of the BDeu score of the network structure.
- measureMDLScore: log of the MDL score.
- measureAICScore: log of the AIC score.
- measureEntropyScore:log of the entropy.

11 Adding your own Bayesian network learners

You can add your own structure learners and estimators.

Adding a new structure learner

Here is the quick guide for adding a structure learner:

- Create a class that derives from weka.classifiers.bayes.net.search.SearchAlgorithm.
 If your searcher is score based, conditional independence based or cross validation based, you probably want to derive from ScoreSearchAlgorithm,
 CISearchAlgorithm or CVSearchAlgorithm instead of deriving from SearchAlgorithm directly. Let's say it is called
 weka.classifiers.bayes.net.search.local.MySearcher derived from
 ScoreSearchAlgorithm.
- 2. Implement the method

public void buildStructure (BayesNet bayesNet, Instances instances). Essentially, you are responsible for setting the parent sets in bayesNet. You can access the parentsets using bayesNet.getParentSet(iAttribute) where iAttribute is the number of the node/variable.

To add a parent iParent to node iAttribute, use bayesNet.getParentSet(iAttribute).AddParent(iParent, instances) where instances need to be passed for the parent set to derive properties of the attribute.

Alternatively, implement public void search (BayesNet bayesNet, Instances instances). The implementation of buildStructure in the base class This method is called by theSearchAlgorithm will call search after initializing parent sets and if the InitAsNaiveBase flag is set, it will start with a naive Bayes network structure. After calling search in your custom class, it will add arrows if the MarkovBlanketClassifier flag is set to ensure all attributes are in the Markov blanket of the class node.

- 3. If the structure learner has options that are not default options, you want to implement public Enumeration listOptions(), public void setOptions(String[] options), public String [] getOptions() and the get and set methods for the properties you want to be able to set.
 - NB 1. do not use the -E options since that is reserved for the BayesNet class to distinguish the extra options for the SearchAlgorithm class and the Estimator class. If the -E option is used, it will not be passed to your SearchAlgorithm (and probably causes problems in the BayesNet class).
 - NB 2. make sure to process options of the parent class if any in the get/setOpions methods.
- 4. Add an entry to weka/gui/GenericObjectEditor.props so that the class shows up when selecting a structure learner. Just add the name of the class

weka.classifiers.bayes.net.search.local.MySearcher to the item weka.classifiers.bayes.net.search.SearchAlgorithm.

Adding a new estimator

This is the quick guide for adding a new estimator:

- Create a class that derives from weka.classifiers.bayes.net.estimate.BayesNetEstimator. Let's say it is called weka.classifiers.bayes.net.estimate.MyEstimator.
- 2. Implement the methods public void initCPTs(BayesNet bayesNet), public void estimateCPTs(BayesNet bayesNet), public void updateClassifier(BayesNet bayesNet, Instance instance), and public double[] distributionForInstance(BayesNet bayesNet, Instance instance).
- 3. If the structure learner has options that are not default options, you want to implement public Enumeration listOptions(), public void setOptions(String[] options), public String [] getOptions() and the get and set methods for the properties you want to be able to set.
 - NB do not use the -E options since that is reserved for the BayesNet class to distinguish the extra options for the SearchAlgorithm class and the Estimator class. If the -E option is used and no extra arguments are passed to the SearchAlgorithm, the extra options to your Estimator will be passed to the SearchAlgorithm instead. In short, do not use the -E option.
- 4. Add an entry to weka/gui/GenericObjectEditor.props so that the class shows up when selecting an estimator. Just add the name of the class weka.classifiers.bayes.net.estimate.MyEstimator to the item weka.classifiers.bayes.net.estimate.BayesNetEstimator.

12 FAQ

How do I use a data set with continuous variables with the BayesNet classes?

Use the class weka.filters.unsupervised.attribute.Discretize to discretize them. From the command line, you can use

java weka.filters.unsupervised.attribute.Discretize -B 3 -i infile.arff -o outfile.arff

where the -B option determines the cardinality of the discretized variables.

How do I use a data set with missing values with the BayesNet classes?

You would have to delete the entries with missing values or fill in dummy values.

How do I create a random Bayes net structure?

Running from the command line

java weka.classifiers.bayes.net.BayesNetGenerator -B -N 10 -A 9 -C $^{\circ}$

will print a Bayes net with 10 nodes, 9 arcs and binary variables in XML BIF format to standard output.

How do I create an artificial data set using a random Bayes nets?

Running

java weka.classifiers.bayes.net.BayesNetGenerator -N 15 -A 20 -C 3 -M 300

will generate a data set in arff format with 300 instance from a random network with 15 ternary variables and 20 arrows.

How do I create an artificial data set using a Bayes nets I have on file?

Running

java weka.classifiers.bayes.net.BayesNetGenerator -F alarm.xml -M 1000 will generate a data set with 1000 instances from the network stored in the file alarm.xml.

How do I save a Bayes net in BIF format?

GUI: In the explorer,

- o learn the network structure,
- o right click the relevant run in the result list,
- o choose Visualize Graph in the pop up menu,
- o click the floppy button in the Graph Visualizer window. o a file "save as" dialog pops up that allows you to select the file name to save to.

Java: Create a BayesNet and call BayesNet.toXMLBIF03() which returns the Bayes network in BIF format as a String.

Command line: Cannot be done (yet).

How do I compare a network I learned with one in BIF format?

Specify the -B
bif-file> option to BayesNet. Calling toString will produce a summary of extra, missing and reversed arrows. Also the divergence between the network learned and the one on file is reported.

How do I use the network I learned for general inference?

There is no general purpose inference in Weka, but you can export the network as XML BIF file (see above) and import it in other packages, for example JavaBayes available under GPL from http://www.cs.cmu.edu/~javabayes.

13 Future development

If you would like to add to the current Bayes network facilities in Weka, you might consider one of the following possibilities.

• Implement more search algorithms, in particular,

- general purpose search algorithms (such as an improved implementation of genetic search).
- structure search based on equivalent model classes.
- implement those algorithms both for local and global metric based search algorithms.
- implement more conditional independence based search algorithms.
- Allow BayesNets to be saved in XML BIF format from the command line.
- Implement score metrics that can handle sparse instances in order to allow for processing large datasets.
- Implement traditional conditional independence tests for conditional independence based structure learning algorithms.
- Currently, all search algorithms assume that all variables are discrete.
 Search algorithms that can handle continuous variables would be interesting.
- A limitation of the current classes is that they assume that there are no missing values. This limitation can be undone by implementing score metrics that can handle missing values. The classes used for estimating the conditional probabilities need to be updated as well.
- Only leave-one-out, k-fold and cumulative cross validation are implemented. These implementations can be made more efficient and other cross validation methods can be implemented, such as Monte Carlo cross validation and bootstrap cross validation.
- Implement methods that can handle incremental extensions of the data set for updating network structures.

And for the more ambitious people, there are the following challenges.

- Allow learning of other graphical models, such as chain graphs, undirected graphs and variants of causal graphs.
- Allow learning of networks with latent variables.
- Allow learning of dynamic Bayesian networks so that time series data can be handled.

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