Published in final edited form as:

Proc Int Conf Mach Learn Appl. 2014 December ; 2014: 362–366. doi:10.1109/ICMLA.2014.64.

ExpertBayes: Automatically refining manually built Bayesian networks

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Abstract

Bayesian network structures are usually built using only the data and starting from an empty network or from a naïve Bayes structure. Very often, in some domains, like medicine, a prior structure knowledge is already known. This structure can be automatically or manually refined in search for better performance models. In this work, we take Bayesian networks built by specialists and show that minor perturbations to this original network can yield better classifiers with a very small computational cost, while maintaining most of the intended meaning of the original model.

Keywords

bayesian networks; advice-based systems; learning bayesian network structures

1 Introduction

Bayesian networks are directed acyclic graphs that represent dependencies between variables in probabilistic models. In these networks, each node represents a variable of interest and the edges may represent causal dependencies between these variables. A Bayesian network encodes the Markov assumption that each variable is independent of its non-descendants, given just its parents. Each node (variable) is associated with a conditional probability table.

When used for knowledge representation, a network is simply a graphical model that represents relations among variables. This graphical model can be learned from data or can be manually built. In the latter case, the network encodes the knowledge of an expert and can serve as a basis for the construction of new networks. When learned only from data, the final graphical model (network structure) may not have a meaning for a specialist in the domain defined by the data.

In this work, we aim to gather the advantages of manual construction with the advantages of automatic construction, using ExpertBayes, a system that implements an algorithm that can refine previously built networks. ExpertBayes allows for (1) reducing the computational

costs involved in building a network only from the data, (2) embedding knowledge of an expert in the newly built network and (3) manual building of fresh new graphical representations. The main ExpertBayes algorithm is random and implements 3 operators: insertion, removal and reversal of edges. In all cases, nodes are also chosen randomly.

Our expert domains are prostate cancer and breast cancer. We used graphical models manually built by specialists as starting networks. Parameters are learned from the data, but can also be given by the specialists. We compare the performance of our original networks with the best network found using our random algorithm. Results are validated using 5-fold cross-validation. For different threshold values, results, both in the training and test sets, show that there is a statistically significant difference between the original network and the newly built networks. As far as we know, this is the first implementation of an algorithm capable of constructing Bayesian networks from prior knowledge in the form of a network structure. Previous works considered as initial network a naïve Bayes or an empty network [10,12,14,5]. As far as we know, the R package deal [2] is the only one that refines previous Bayesian structures, but our attempts to make it work were not successful, since the parameters computed for the new networks were not interpretable. We then decided to implement our own algorithm.

One important aspect of ExpertBayes is that it makes small perturbations to the original model thus maintaining its intended meaning. Besides refining pre-defined networks, ExpertBayes is interactive. It allows users to play with the network structure which is an important step in the integration of expert knowledge to the automatic learning process.

2 ExpertBayes: refining expert-based Bayesian networks

Most works in the literature that discuss methods for learning the structure of Bayesian networks focus on learning from an empty network or from data. However, in some domains, it is common to find Bayesian models manually built by experts, using tools such as GeNIe (a modeling environment developed by the Decision Systems Laboratory of the University of Pittsburgh, available at http://genie.sis.pitt.edu), Netica (https://www.norsys.com/netica.html) or the WEKA Bayes editor [10]. Having an initial model brings at least two advantages: (1) from the point of view of the specialist, some expert knowledge has already being embedded to the model, with meaningful correlations among variables, (2) from the point of view of the structure learning algorithm, the search becomes less costly, since an initial structure is already known. In fact, in other areas, it is very common to use previous knowledge to reduce the search space for solutions. One classical example is the comb-like structure used as initial seed for DNA reconstruction algorithms based on Steiner minimum trees. In the past, the protein structure was searched for from an empty initial structure [15]. The discovery that most protein structures in the nature had a comb-like shape reduced the algorithm cost allowing to solve much bigger problems [11].

ExpertBayes uses a simple, yet efficient algorithm to refine the original network. This algorithm is shown in Figure 20. It reads the initial input network and training and test sets. It then uses a standard method to initialize the probability tables, by counting the case frequency of the training set for each table entry. Having the prior network and conditional

probability tables, the algorithm makes small perturbations to the original model. It first chooses a pair of nodes, then it randomly chooses to add, remove or revert an edge. If the operation is to add an edge, it will randomly choose the edge direction. Operations are applied if no cycle is produced. At each of these steps, conditional probability tables are updated, if necessary, i.e., if any node affected belongs to the Markov blanket of the classifier node. A score of the new model is calculated for the training set and only the best pair network/score is retained when the repeat cycle ends. This best network is then applied to the test set (last step, line 20 of the algorithm). A global score metrics is used, the number of correctly classified instances, according to a threshold of 0.5.

Algorithm 1

ExpertBayes

Data:
OriginalNet, *// initial network structure*;
Train *// training set*;
Test *// test set*
Result:
scoreTrain *// scores in the training set for BestNet*
scoreTest *// scores in the test set for BestNet*
BestNet *// best scored network on Train*

```
1  Read OriginalNet;
2  Read Train and Test sets;
3  BestNet = OriginalNet;
4  Learn parameters for OriginalNet from training set;
5  repeat
6      Randomly choose a pair of nodes N1 and N2;
7      if there exists an edge between N1 and N2 then
8          randomly choose: revert or remove
9      else
10         choose add operation;
11         randomly choose edge direction
12     end
13     Apply operation to OriginalNet obtaining NewNet;
14     Rebuild necessary CPT entries, if necessary;
15     Compute scoreTrain of the NewNet;
16     if scoreTrain NewNet > scoreTrain BestNet then
17         BestNet = NewNet
18     end
19 until N iterations using OriginalNet and Train;
20 Apply BestNet to Test and compute scoreTest;
```

The modifications performed by ExpertBayes are always over the original network. This was strategically chosen in order to cause a minimum interference on the expert knowledge represented in the graphical model. ExpertBayes has also the capability of creating a new network only from the data if the user has no initial network to provide.

3 Materials and Methods

The manual construction of a Bayesian network can be tedious and time-consuming. However, the knowledge encoded in the graphical model and possibly in the prior probabilities is very valuable. We are lucky enough to have two of these networks. One was built for the domain of prostate cancer and the second one was built for breast cancer.

In the prostate cancer domain, variables were collected [13] taking into account three different moments in time: (1) during a medical appointment, (2) after auxiliary exams are performed and (3) five years after a radical prostatectomy. Such variables are age, weight, family history, systolic and diastolic arterial blood pressure, hemoglobin rate, hypoecogenic nodules, prostate specific-antigen (psa), clinical status, doubling time PSA, prostate size, among others. Five years after the surgery, we assess morbidity for those patients.

The data for breast cancer was collected from patients of the University of Wisconsin Medical Hospital. Mammography features were annotated according to the BI-RADS (Breast Imaging and Data Reporting System) [4]. These include breast density, mass density, presence of mass or calcifications and their types, architectural distortion, among others. One variable indicates the diagnostic and can have values malignant or benign, to indicate the type of finding.

A third set of data was used, also with mammographic features from the University of Wisconsin Medical Hospital, but with a different set of patients and a smaller number of variables.

3.1 Original Bayesian Networks

Two of our networks were built by specialists while the third one was built by us. The Bayesian networks built by our specialists are shown in Figures 1 [13] and 2 [3].

We call them Original Networks. Both of them were built by specialists in prostate cancer and breast cancer using high risk and low risk factors mentioned in the literature and their own experience. Prior probabilities are taken from the training data. The class variable for the breast cancer data is CatDx. In other words, the classifying task is to predict a malignant or benign finding. The class variable for the prostate cancer data is the life expectancy five years after the surgery, called class in Figure 1.

The third network was also manually built using the model of Figure 2 as a basis, but with a smaller set of features used in another work [8]. The class variable is Outcome with values malignant or benign.

3.2 Datasets

The characteristics of the datasets used are shown in Table 1. The three of them have only two classes. For Breast Cancer (1) and Breast Cancer (2), the Pos column indicates the number of malignant cases and the Neg column indicates the number of benign cases. For Prostate Cancer, the Pos column indicates the number of patients that did not survive 5 years after surgery.

The dataset for Prostate Cancer is available from http://lib.stat.cmu.edu/S/Harrell/data/descriptions/prostate.html [1].

For each one of the datasets, variables with numerical values were discretized according to reference values in the domain (for example, variables such as age and size are discretized in intervals with a clinical meaning). The same discretized datasets were used with all algorithms.

3.3 Methodology

We used 5-fold cross-validation to train and test our models. We compared the score of the original network with the score of ExpertBayes. We also used WEKA [10] to build the network structure from the data with the K2 [7] and TAN [9] algorithms. K2 is a greedy algorithm that, given an upper bound to the number of parents for a node, tries to find a set of parents that maximizes the likelihood of the class variable. TAN (Tree Augmented Naïve Bayes) starts from a naïve Bayes structure where the tree is formed by calculating the maximum weight spanning tree using Chow and Liu algorithm [6]. In practice, TAN generates a tree over naïve Bayes structure, where each node has at most two parents, being one of them the class variable. We ran both algorithms with default values and both start from a naïve Bayes structure. The best networks found are shown and contrasted to the original network and to the network produced by ExpertBayes.

4 Results

In this Section, we present the results measured using CCI (percentage of Correctly Classified Instances) and Precision-Recall curves. Precision-Recall curves are less sensitive to imbalanced data which is the case of our datasets. We also discuss about the quality of the generated networks.

4.1 Quantitative Analysis

CCI Table 2 shows the results (Correctly Classified Instances - CCI) for each test set and each network. Results are shown in percentages and are macro-averaged across the five folds. All results are shown for a probability threshold of 0.5.

For the Prostate Cancer data, ExpertBayes is better than WEKA-TAN with $p < 0{:}01$. The difference is not statistically significant between the ExpertBayes and the Original Network results and ExpertBayes and WEKA-K2.

With $p < 0{:}004$, for Breast Cancer (1), ExpertBayes produces better results than the Original Network (63% CCI against 49% CCI of the original network). With the same p-value, ExpertBayes (63% CCI) is also better than WEKA-K2 (59%). With $p < 0{:}002$, ExpertBayes is better than WEKA-TAN (57%).

For Breast Cancer (2), WEKA-K2 is better than ExpertBayes with $p < 0{:}003$. WEKA-TAN is also better than ExpertBayes with $p < 0{:}008$. ExpertBayes is only better than the original network, with $p < 0{:}009$.

Recall that these results are achieved with a threshold of 0.5.

Precision-Recall Analysis—Instead of looking only at CCI with a threshold value of 0.5, we also plotted Precision-Recall curves. Figure 4 shows the curves for the three datasets. Results are shown for the test sets after cross-validation. We used values of 0.02 and 0.1 (threshold values commonly used in clinical practice for mammography analysis) and also varied the thresholds in the interval 0.2–1.0.

The baseline precision for the three datasets are: 71% for Prostate Cancer, 55% for Breast Cancer (1) and 37% for Breast Cancer (2). These baseline values correspond to classifying every case as belonging to one class. For Breast Cancer (1) and Breast Cancer (2), this class is malignant. For Prostate Cancer, the class is not survival.

The first important conclusion we can take from these curves is that ExpertBayes is capable of improving Precision over the other models, at the same Recall level. In practice, this means that a smaller number of healthy patients will be sent to inconvenient procedures in the case of breast cancer analysis and a smaller number of patients will have a wrong prognostic of not survival after 5 years of surgery for the Prostate cancer analysis.

The second conclusion we can take is that expert-based models applied to data produce better performance than the traditional network structures built only from the data. This means that expert knowledge is very useful to help giving an initial efficient structure. This happened to all datasets.

A third conclusion we can take is that a small set of features can have a significant impact on the performance of the classifier. If we compare Figure 4b with Figure 4c, all classifiers for Breast Cancer (2) outperform the classifiers of Breast Cancer (1). This may indicate that to prove malignancy, an expert need to look at a fewer number of features.

One caveat, though, needs to be avoided. If we look at the performance of the model produced by ExpertBayes for Breast Cancer (1), this is perfect for a given threshold, with maximum Recall and maximum Precision. This can happen when variables are highly correlated as is the case of Disease and CatDx. In our experiments, WEKA did not capture this correlation because the initial network used is a naïve structure (no variable ever has an edge directed to the class variable). As we allow edge reversal, the best network found is exactly one where Disease has an edge directed to the CatDx class variable. However, this is an excellent opportunity to the interactive aspect of ExpertBayes, since the expert now can notice that this happens and can remove one of the nodes or prevent the reverted correlation from happening.

4.2 Bayes Networks as Knowledge Representation

Examples of the best networks produced by ExpertBayes and WEKA-K2 and WEKA-TAN are shown in Figure 5 for Prostate Cancer and in Figures 6 and 7 for Breast Cancer (1) and Breast Cancer (2).

The best networks produced by ExpertBayes maintain the original structure with its intended meaning and show one single modification to the original model by adding, removing or reversing an edge. For example, for Prostate Cancer, Figure 5a, a better network was

produced that shows a relation between the diastolic blood pressure (dbp) and the class variable. It remains to the specialist to evaluate if this has some clinical meaning. For Breast Cancer (1), the best network is found when a correlation is established between MassMargins and the class variable (Figure 6a). It is well known from the literature in breast cancer that some BI-RADS factors are very indicative of malignancy and MassMargins is one of them. For Breast Cancer (2) (Figure 7a, the best network produced by ExpertBayes has an added edge between MassShape and Outcome, indicating that besides Age and BreastDensity, MassShape has also some influence on the class variable.

Results produced with the WEKA tool show networks very different from the ones built by experts. This was expected since the model is built only from the data and not all possible networks are searched for due to the complexity of searching for all possible models. The K2 algorithm found that the best model for all datasets was the naïve Bayes model. Both models produced using K2 and TAN convey another meaning to the specialist that is quite different from the initial intended meaning. This happened with all networks produced by WEKA, for both datasets.

5 Conclusions

We implemented a tool that can allow the probabilistic study of manually built bayesian networks. ExpertBayes is capable of taking as input a network structure, learn the initial parameters, and iterate, producing minor modifications to the original network structure, searching for a better model while not interfering too much with the expert knowledge represented in the graphical model. ExpertBayes makes small modifications to the original model and obtain better results than the original model and better than models learned only from the data. Building a Bayesian network structure from the data or from a naïve Bayes structure is very time-consuming given that the search space is combinatorial. ExpertBayes takes the advantage of starting from a pre-defined structure. In other words, it does not build the structure from scratch and takes advantage of expert knowledge to start searching for better models. Moreover, it maintains the basic structure of the original network keeping its intended meaning. ExpertBayes is also an interactive tool with a graphical user interface (GUI) that allows users to play with their models thus exploring new structures that give rise to a search for other models. We did not stress this issue in this work as our focus was on showing that ExpertBayes can refine well pre-defined models. Our main goal for the future is to improve the algorithm in order to have better prediction performance, possibly using more and quality data and different search and parameter learning methods. We also intend to embed in Expert-Bayes a detection of highly correlations that exist among variables to warn the expert. If this is done before learning we could avoid producing unnecessary interactions between the user and the system.

Acknowledgments

This work was partially funded by projects ABLe (PTDC/ EEI-SII/ 2094/ 2012), ADE (PTDC/EIA-EIA/ 121686/2010) and QREN NLPC Coaching International 38667 through FCT, COMPETE and FEDER and R01LM010921: Integrating Machine Learning and Physician Expertise for Breast Cancer Diagnosis from the National Library of Medicine (NLM) at the National Institutes of Health (NIH).

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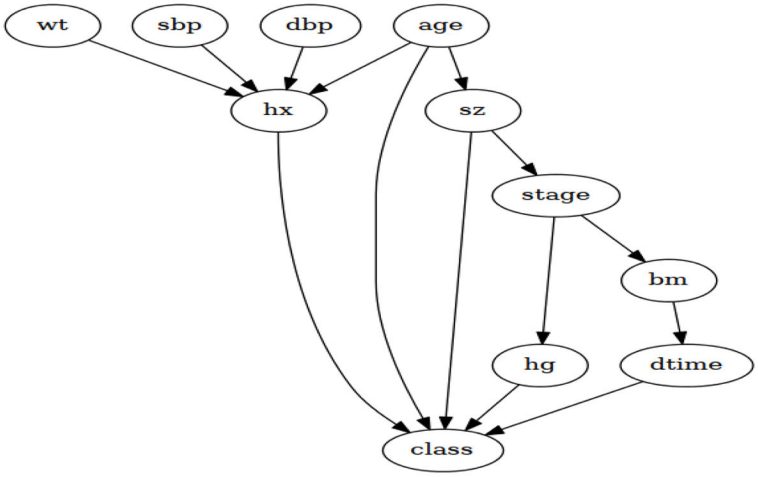


Fig. 1.
Original Network Model for Prostate Cancer

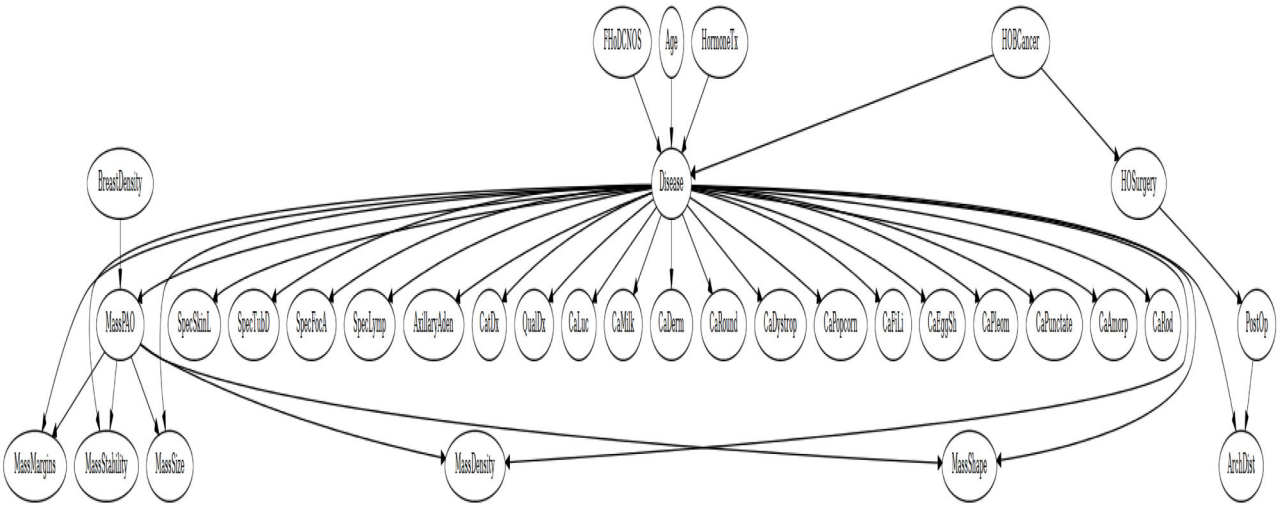


Fig. 2.
Original Network Model for Breast Cancer (1)

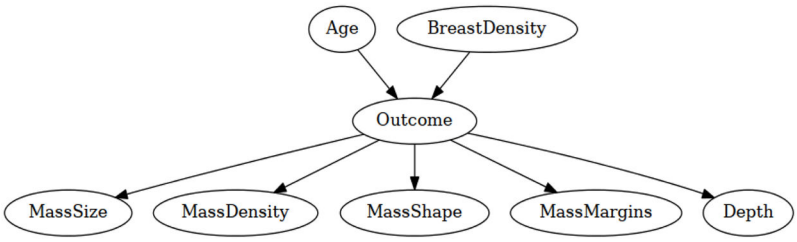
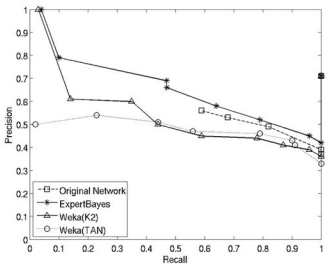
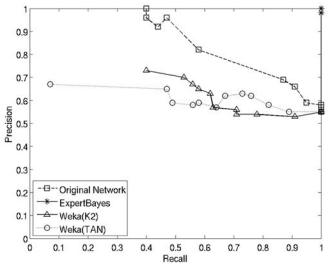


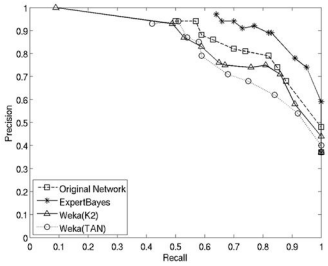
Fig. 3.
Original Network Model for Breast Cancer (2)



(a) Prostate

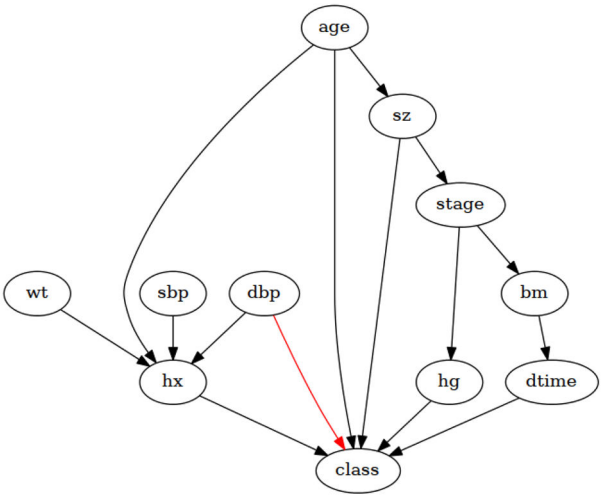


(b) Breast Cancer (1)

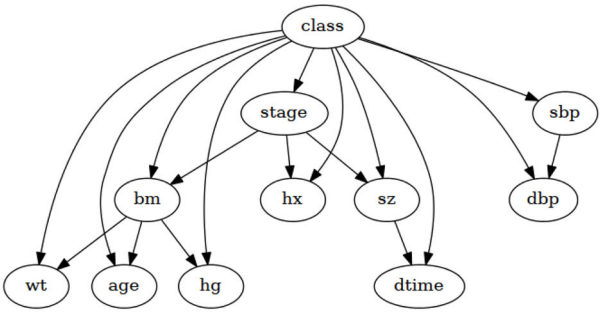


(c) Breast Cancer (2)

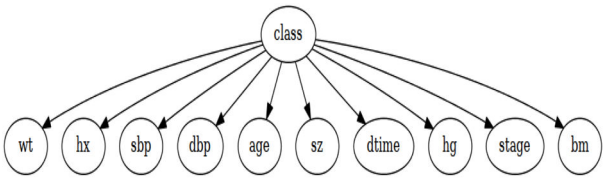
Fig. 4.
Precision-Recall Curves for various thresholds



(a) ExpertBayes



(b) WEKA-TAN



(c) WEKA-K2

Fig. 5.
Best Models for Prostate Cancer

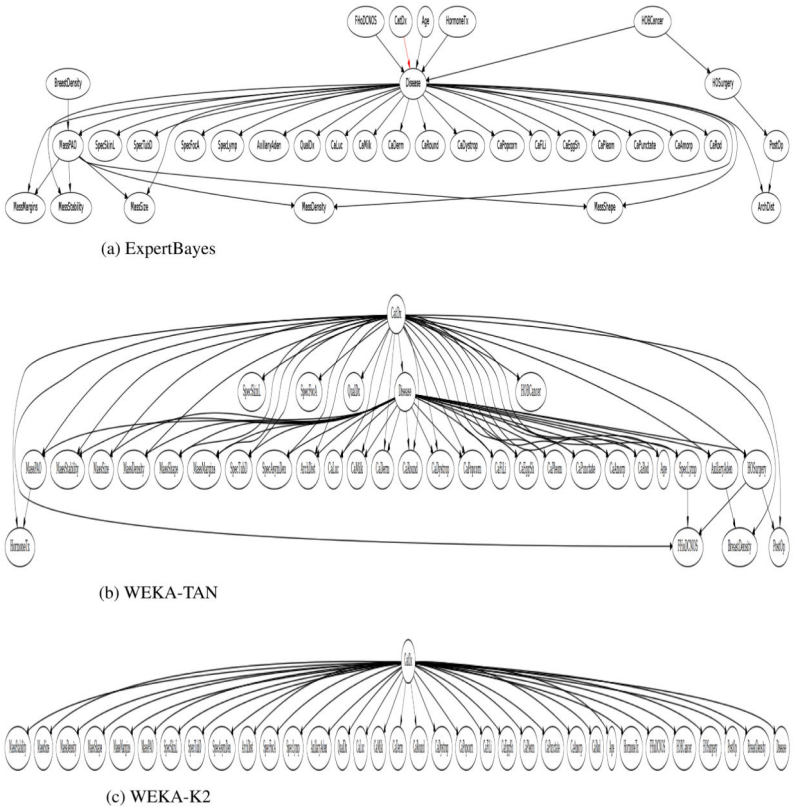
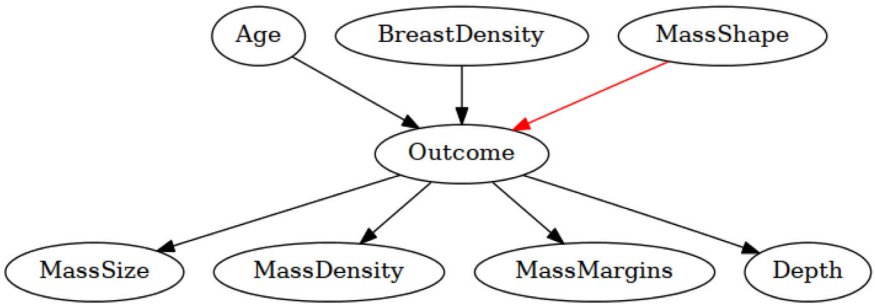
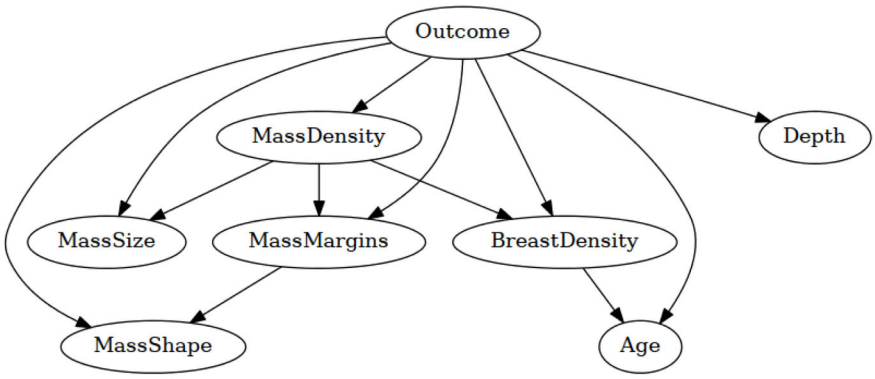


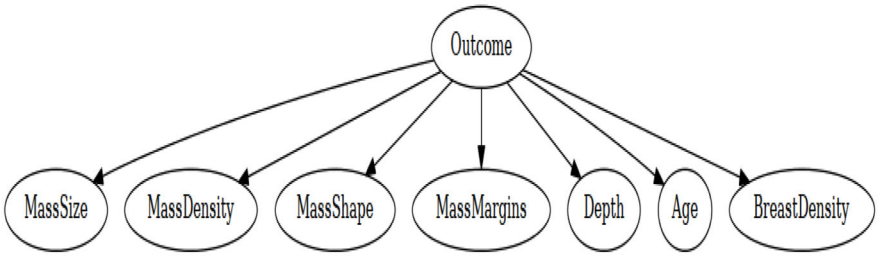
Fig. 6.
Best Models for Breast Cancer (1)



(a) ExpertBayes



(b) WEKA-TAN



(c) WEKA-K2

Fig. 7.
Best Models for Breast Cancer (2)

Table 1

Datasets Descriptions

Dataset	Number of Instances	Number of Variables	Pos	Neg
Prostate Cancer	496	11	352	144
Breast Cancer (1)	100	34	55	45
Breast Cancer (2)	241	8	88	153

Table 2

CCI test set - averaged across 5-folds

Dataset	Original	ExpertBayes	WEKA-K2	WEKA-TAN
Prostate Cancer	74	76	74	71
Breast Cancer (1)	49	63	59	57
Breast Cancer (2)	49	64	80	79