Dependency detection with Bayesian Networks

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1. Introduction

Most methods aimed to detect dependency between two variables do not consider interventions with numerous other variables and often make groundless assumptions about relation form. Bayesian networks help to despise of the drawbacks. Bayesian networks allow one to learn about causal relationships. Bayesian networks can consider prior knowledge. Bayesian networks can readily handle incomplete data sets.

A Bayesian network is a probabilistic graphical model (a type of statistical model) that represents a set of random variables and their conditional dependencies via a directed acyclic graph (DAG). For a long time Bayesian networks were used as a representation for encoding uncertain expert knowledge in expert systems. Recently, methods were developed to learn Bayesian network from data. Nowadays data analysis bring up a problem of learning a Bayesian network structure. This work is dedicated to finding the scope of data dependencies modern applied algorithms can detect with Bayesian networks. Specifically, experiments aimed to detect dependency between two variables were done with the use of pebl library[2].

In section 2, there are a few more words about what a Bayesian network is. In section 3, we present a Python package pebl and discuss pebl implemented tools for structure learning and probabilities learning in a fixed Bayesian-network structure. In section 4, testing of pebl tools and experiments on how well pebl detects dependencies are presented.

2. Bayesian Network graphical model

Formally, Bayesian networks are DAGs whose nodes represent random variables. Edges represent conditional dependencies; nodes that are not connected represent variables that are conditionally independent of each other. That also means that absence of an edge between two nodes doesn't really mean actual independence between corresponding variables, because they can influence each other through other variables. Each node is associated with a probability function that takes, as input, a particular set of values for the node's parent variables, and gives the probability distribution of the variable represented by the node. For example, if m parent nodes represent m Boolean variables then the probability function could be represented by a table of 2^m entries, one entry for each of the 2^m possible combinations of its parents being true or false (see example on Figure 1).

In order to fully specify the Bayesian network it is necessary to define the joint probability distribution of the statistical model, thus to specify for each node X the probability distribution for X conditional upon X's parents. It may have any form. In this work discrete distribution is used since it simplifies calculations. In a situation when only constraints on a distribution are

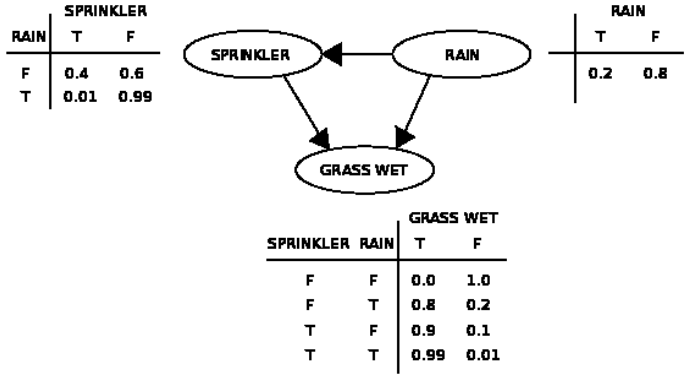

Figure 1. A simple Bayesian network and its conditional probability tables. The joint probability is $\mathrm{P}(G, S, R) = \mathrm{P}(G|S, R)\mathrm{P}(S|R)\mathrm{P}(R)$, where G correspond to Grass Wet variable, S – Sprinkler, R – Rain.

known, the principle of maximum entropy can help to determine the distribution. It will be a distribution that both maximizes entropy and meet the constraints.

Often these conditional distributions include parameters which are unknown and must be estimated from data, sometimes using the maximum likelihood approach. Direct maximization of the likelihood (or of the posterior probability) is often complex when there are unobserved variables. A classical approach to this problem is the expectation-maximization algorithm which alternates computing expected values of the unobserved variables conditional on observed data, with maximizing the complete likelihood (or posterior) assuming that previously computed expected values are correct.

In the simplest case, a Bayesian network is specified by an expert and is then used to perform inference. But commonly the task of defining the network is too complex for humans. Then the network structure and the parameters of the local distributions must be learned from data.

The common approach to structural learning is to introduce a statistically motivated scoring function that evaluates each network with respect to the training data and to search for the optimal network according to this score. For a scoring function posterior probability of the structure given the training data can be used. The exhaustive maximization of the score is known to be an NP-hard problem. Thus heuristic search is often used.

3. Pebl library

In this paper, we introduce pebl, a Python library and application for learning Bayesian network structure from data. Although learning the structure of BNs from data is now common, there are still a few high-quality open-source softwares that can meet the needs of various users. End users require software that is easy to use; supports learning with different data types; can accommodate missing values and hidden variables; and can take advantage of various computational clusters and grids. Pebl is the Python Environment for Bayesian Learning to meet these needs.

3.1. Functionality

pebl:

- can work with continuous, discrete and categorical variables (with different type variables simultaneously);
- can perform maximum entropy discretization (that is when single variable values are compressed into fixed number of bins according to maximum entropy criterion);
- uses the BDe metric for scoring networks and handles interventional data using the method described in [4];
- can handle missing values and hidden variables using exact marginalization and Gibbs sampling [1];

	BANJO	BNT	Causal Explorer	Deal	LibB	PEBL
License	Academic	GPL	Academic	GPL	Academic	MIT
Scripting language	Matlab	Matlab	Matlab	R	N/A	Python
Interventional Data	No	Yes	No	No	No	Yes
Dynamic BN	Yes	Yes	No	No	No	No
Structural Priors	Yes	No	No	No	No	Yes
Missing Data	No	Yes	No	No	Yes	Yes
Parallel Execution	No	No	No	No	No	Yes

Table 1. Popular Bayesian network structure learning software.

- supports structural priors over edges specified as "hard" constraints or "soft" energy matrices (see [5] for details, this option was not used in our experiments) and arbitrary constraints specified as Python functions or lambda expressions.

3.2. pebl interface use

- In the input data file type of variables should be specified;
- Apply `pebl.data.discretize(num_bins)` to compress unique values of continuous or discrete variables to `num_bins` number of values (so pebl sees continuous variables as discrete);
- For parallel calculations use `pebl.multiprocess`;
- `pebl.result.post[:10]` is made to access top score network configurations and `pebl.result.cons` to access its consensus matrix C (where C_{ij} is a p-value referring to an edge from i-th to j-th node).

3.3. Convenience and Scalability

While many tasks related to Bayesian learning are embarrassingly parallel in theory, few software packages take advantage of it. pebl can execute learning tasks in parallel over multiple processors or CPU cores.

With appropriate configuration settings and the use of parallel execution, pebl can be used for large learning tasks. Although pebl has been tested successfully with datasets with 10000 variables and samples, BN structure learning is a known NP-Hard problem [6] and analysis using datasets with more than a few hundred variables is likely to result in poor results due to poor coverage of the search space.

3.4. Related Software Comparison

While there are many software tools for working with BNs, most focus on parameter learning and inference rather than structure learning. As shown in Table 1, the ability to handle interventional data, model with missing values, use soft and arbitrary priors and exploit parallel platforms are unique to pebl. pebl, however, does not currently provide any features for learning Dynamic Bayesian Networks (a Bayesian Network which relates variables to each other over adjacent time steps). Also pebl can be slower than software written in C/C++ or Java, because it uses Python libraries, but still pebl benefits from parallel learning and edge prior implementation, making itself applicable to a wider range of problems than other software.

4. Experiments

In the section there are different tests of pebl dependency detection abilities. To check if a program detects dependency between two variables or not we use as input features reflected

Feature	Name	Values
main feature	x	$\mathcal{N}(2, 10)$
dependency	f(x)	f(x)
independable feature	y	$\mathcal{N}(2, 10)$

Table 2. Features to detect dependency $x \to f(x)$.

in Table 2. Since an output of pebl learner consists of top scoring networks and a consensus matrix, we use minimum p-value of edges we expect to be present and maximum p-value of all edges connecting independent features to verify algorithm answer. An edge p-value is a rate of top scored networks containing the edge. Best p-value an edge can have is 1 and the lowest is 0. So p-value represents probability of the edge presence in the optimal structure of BN for the variables.

Bayesian network do not comprise cycles, so dependencies like linear relation can be represented with two structures (see Figure 2).

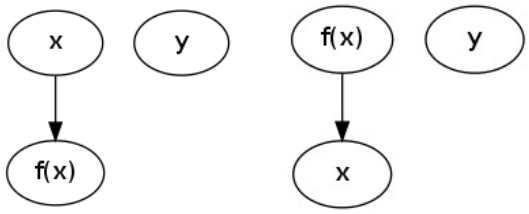

Figure 2. For most functions f(x) these are equivalent structures.

Maximum entropy discretization plays an important role in dependency detection. Given x, y and $f(x + n_1) + n_2$, $n_1 \sim \mathcal{N}(0, 0.2)$, $n_2 \sim \mathcal{N}(0, 0.1)$ we variate `num_bins` and check how p-values of "true" edges (those connecting dependable features) change. Our dataset consists of 100 objects. On Figure 3 p-values of "true" edges exceed p-values of "false" edges (those connecting independable features) in the (35; 38) and (50, 75) `num_bins` intervals, that is where dependency $x \to f(x)$ is detected. "65" value seems the most certain.

How to detect optimal `num_bins` value without knowing true edges?

- On Figure 3 p-values of "false" and "true" edges are reflected. The regions where "false" p-values are nonzero is where network fails to recognise independence. So it will be best to select `num_bins` value, where network is more confident in "true" edges than in "false" ones (for example, `num_bins` $\in [55, 75]$).

Finally we noise data with normal distributed variable to inspect limits of pebl linear dependency detection ability. The dependency is recognised quite well (Figure 4), see example of noised data in Figure 5.

Polynomial dependency detection is reflected on Figures 6, 7.

On Figures 3 and 6 it is worth noticing that 0.5 is a frequent value for "true" edges p-value and also it's upper limit. Dependency configurations $x \to f(x)$ and $f(x) \to x$ appear in top score networks same number of times and each of their p-value will be 0.5. That proves our assumption about equivalence of the configurations.

5. Conclusion

We introduced Bayesian network library pebl, reviewed it's implemented tools and made several suggestions on how to work with pebl. Experiments show that for two variables dependency detection it works much better than a man's eye. With the use of parallel calculations Bayesian networks structure-learners can be a powerful dependency detection tool.

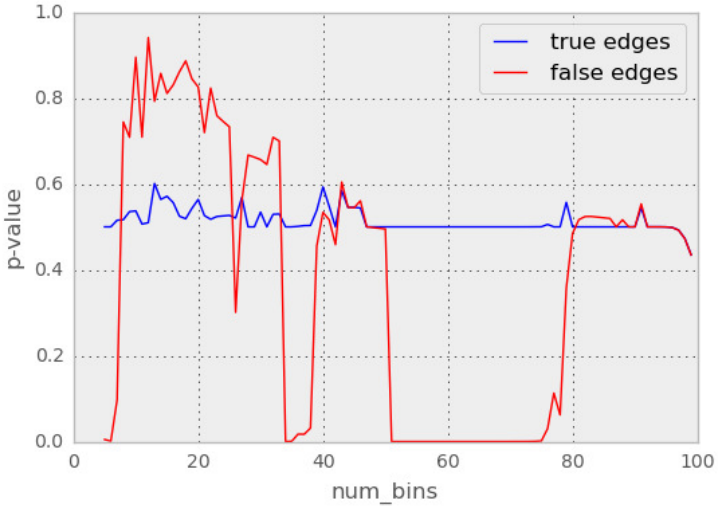

Figure 3. Edges p-values (varying num_bins) for linear dependency dataset.

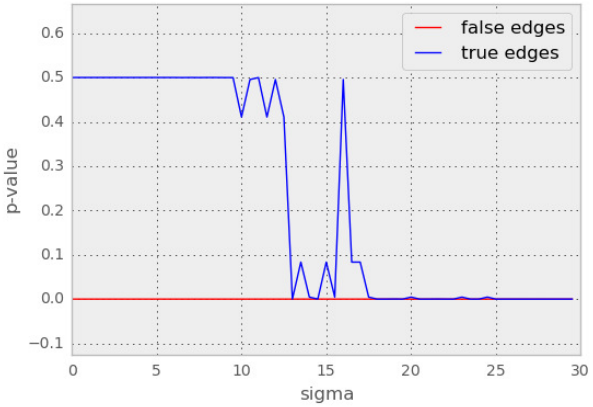

Figure 4. Edges p-values (varying noise$\sim \mathcal{N}(0, sigma)$) for linear dependency dataset.

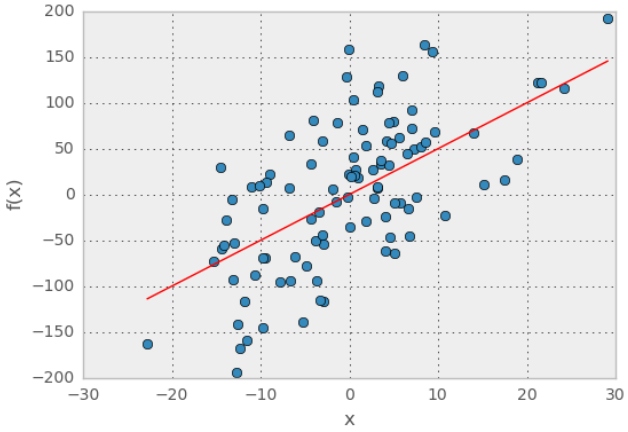

Figure 5. Linear dataset with noise sigma=10.

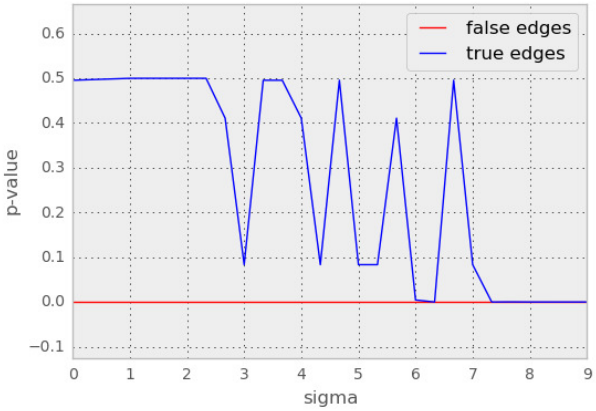

Figure 6. Edges p-values (varying noise$\sim \mathcal{N}(0, sigma)$) for polynomial dependency dataset.

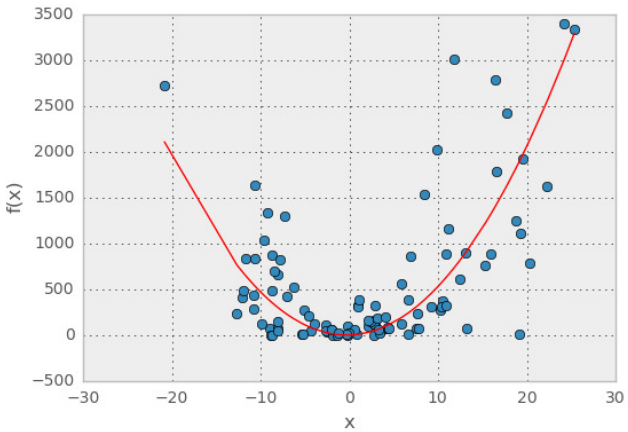

Figure 7. Polynomial dataset with noise sigma=5.

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