Information-Theoretic Scoring Rules to Learn Additive Bayesian Network Applied to Epidemiology

Gilles Kratzer
Department of Mathematics
University of Zurich
Zurich, Switzerland

Reinhard Furrer
Department of Mathematics
Department of Computational Science
University of Zurich
Zurich, Switzerland

August 6, 2018

Abstract
Bayesian network modelling is a well adapted approach to study messy and highly correlated datasets which are very common in, e.g., systems epidemiology. A popular approach to learn a Bayesian network from an observational datasets is to identify the maximum a posteriori network in a search-and-score approach. Many scores have been proposed both Bayesian or frequentist based. In an applied perspective, a suitable approach would allow multiple distributions for the data and is robust enough to run autonomously. A promising framework to compute scores are generalized linear models. Indeed, there exists fast algorithms for estimation and many tailored solutions to common epidemiological issues. The purpose of this paper is to present an R package abn that has an implementation of multiple frequentist scores and some realistic simulations that show its
usability and performance. It includes features to deal efficiently with data separation and adjustment which are very common in systems epidemiology.

**Keywords**— Bayesian Network, structure learning, information theoretic score, data separation

1 Introduction and background

Bayesian Network (BN) modelling has an impressive track record in analysing systems epidemiology datasets [2, 18], especially in veterinary epidemiology [2, 6, 17, 19, 25]. It is a particularly well suited approach at the beginning of the coil of discovery within a field of research to better understand the underlying structure of the data. It is designed to sort out directly from indirectly related variables and offers a far richer modelling framework than classical approaches in epidemiology, like, e.g., regression techniques or extensions thereof. In contrast to structural equation modelling [9], which requires expert knowledge to design the model, the Additive Bayesian Network (ABN) method is a data-driven approach [15, 16]. It does not rely on expert knowledge but it can possibly incorporate it.

1.1 Previous work and other implementations

There exists two broad classes of algorithms to learn BNs. The constraint-based approaches, where one learns the BN using statistical independence tests. The optimal network is identified using the reciprocal relationship between graphical separation and conditional independence [28]. An other popular approach is based on network scoring. The idea is that each candidate network is scored and the one which has the largest score is kept. In practice this is computationally intractable for a typical number of variables. Indeed, the number of possible networks is massive and increases super-exponentially with the number of nodes [24]. A practical workaround is to use a decomposable score, i.e., a score that is additive in terms of network’s node and depends only on the parents of the index node. This approach is very close to the classical model selection in statistics [32]. The scoring approach paradigm is that the scores should represents how well the structure fits the data [32]. Many scores have been proposed for discrete BNs in a Bayesian context [3] that aims at maximising the posterior probability.
Indeed Heckerman et al. \cite{11} proposes the so-called the Bayesian Dirichlet (BD) family of scores. It regroups the K2, BDeu, BDs, BDla scores \cite{27}.

On the other hand, scores within a frequentist framework have been proposed \cite{3}, such as Bayesian Information Criterion (BIC), Akaike Information Criterion (AIC), Minimum Description Length (MDL) \cite{3}. They all have in common a goodness-of-fit part and a penalty for model complexity. Indeed, the naive idea to use the maximum likelihood as a score is suboptimal as it generally selects a fully connected graph.

One major limitation of the scoring approach is that many different networks can have the same score. Networks which have the same scores are in the same equivalence class. The BDeu is the only score-equivalent BD score. BDs is only asymptotically score equivalent. One interesting feature is that BIC is also score equivalent for discrete BNs. In a causal perspective, i.e., when arcs direction matters, scores which are equivalent are preferred \cite{27}.

R as an open source, reliable and easy to use environment for statistical computing is very popular in the epidemiological community \cite{23}. One popular R package for BN learning is the package bnlearn \cite{26}. It has implementations of most of BD’s scores but also AIC and BIC for continuous and discrete mixed variables. Additionally, it has implementations of multiple network structure learning via multiple constraint-based and score-based algorithms. Focused on a causal framework, pcalg is very popular \cite{12}. It has an implementation of the PC-Algorithm that selects one class representative of the network skeleton. Other useful R packages are actively maintained on CRAN. But none of them has an implementation of scoring procedure that deals simultaneously for multiple exponential family representative in a likelihood based framework. Beside R, it exists multiple implementation in other computing environment such as Weka \cite{1}, Matlab \cite{21} or open sources python or C++ implementation. But in the epidemiological community the R implementation are the most popular ones due to the simplicity of use of R.

1.2 Motivations for frequentist scoring

One actual strong limitation of the R package ABN is that it cannot deal with multinomial distributed random variables. Indeed, in applied epidemiology, the data are often composed of a mixture of different distributions. The most common are categorical, continuous and discrete random variable. The
R package ABN has an implementation of binomial, Gaussian and Poisson Bayesian regression. This implies that when dealing with categorical random variable one has to split the random variable in a pairs. This is interesting from a modelling perspective as this is very flexible. But it destroys the intrinsic link between the dichotomised variables which can negatively affects the modelling. Additionally, it increases the number of variables which is computationally not desirable.

A surprisingly common problem when dealing with binomial regression in an applied perspective is the so-called data separation problem \cite{8}. This arises when a covariate predicts perfectly the outcome. A related issue is the quasi data separation (or data sparsity), when the number of observation per class is dramatically low. In such configuration, the maximum likelihood estimates tends to diverge and the classical algorithms for estimation becomes numerically unstable. A possible workaround is to exclude predictors that create separation. This is in general a suboptimal idea as those predictors are specifically the ones that are the most promising to explain the outcome \cite{31}. Related approaches would be to exclude specifically cases that are separated, to collapse predictors categories or to bin predictor values. In a machine learning perspective when dealing with a large number of variables and automatised procedures require robustness. Those data tailored workarounds scale laboriously. An other option is to change a few randomly selected observations in order to render the problem estimable. This implies to see separation as a problem per se rather than as a symptom of paucity of information in the data.

In a Bayesian framework, a possible solution is to use the prior to drive the posterior when the likelihood fails to correctly estimate the information contained in the data. This implies to put some information in the prior. In a frequentist approach, one can penalise the likelihood in order to prevent from becoming infinite. This approach, called bias reduction, can be easily implemented in an iterative scheme by generating pseudo data \cite{14}. Surprisingly, this latter approach originally proposed by Firth \cite{7} is equivalent to penalised the log-likelihood using a Jeffreys prior \cite{14}. Due to the simplicity of implementation the bias-reduced estimation was the chosen solution for data separation in ABN.

In epidemiology, statistical adjustment is often used to control for the effect of supposed confounding factors and make comparison according to different populations more easy \cite{30}. ABN has an option to compute statistically adjusted structures. The adjusting variables are imposed as covariate
to every models computed in the cache.

2 Additive Bayesian networks

ABN models are graphical models that extend the usual Generalized Linear Model (GLM) to multiple dependent variables through the factorisation of their joint probability distribution \cite{16}. They are represented with a Directed Acyclic Graph (DAG) and the set of parameter estimates. An ABN model assumes that each node is a GLM where the covariate are the parents and the distribution depends on the index node. The model learning phase is a two steps process: 1. Network, skeleton or structure learning (\(S\)) 2. Parameter learning, the model parameter are \(\theta_M\). Hence in a Bayesian framework, constructing an ABN model \(M\) given a set of data, \(D\) is:

\[
P(M | D) = P(\theta_M, S | D) = P(\theta_M | S, D) \cdot P(S | D) .
\]

The two learning steps are interconnected. Several efficient algorithms have been proposed for both learning procedures. In order to learn the relationships between variables, the conditional probability distributions tables should be learned, this can be done in a frequentist setting using the classical Iterative Reweighed Least Square (IRLS) algorithm \cite{5}. The structure selection step can be done using a heuristic or exact approach.

An interesting feature of the ABN methodology is to be able to impose external expert knowledge. Indeed, in most of applied data analysis, some part of the network is known. For example, if two random variables are timely related the direction of the possible arrow is known. Or if, based on existing literature a possible connection is known to be expected. ABN allows such external causal input through a banning or a retaining matrix. Those matrices are used to compute the list of valid parent combination. However, a more theoretically sounding approach, suggested by Heckerman et al. \cite{11}, is to use augment the observed data with synthetic data that represents the causal belief. This approach is superior as it solves the problem of the likelihood equivalence posed by banning and retaining part of the structure, but its feasibility in an ABN analysis remains an open question \cite{19}.
2.1 Scoring procedure

The crucial points regarding BN learning process is speed and resilience. Indeed, ABN computes autonomously a comprehensive cache of licit scores. More precisely it computes all allowed combinations, i.e. not banned, of a node and his set of parents up to a given complexity ideally without end user involvement.

A popular choice for estimating GLMs is the IRLS algorithm \[5\]. However, IRLS implementations are known to be potentially numerically unstable, mainly due to rank deficiency and we will treated this issue separately. The IRLS algorithm is able to estimate every distribution of the exponential family. The distributions of interest for ABN are: Gaussian, binomial and Poisson. The multi-categorical random variables can be estimated through IRLS like algorithm. But a well known weakness of this approach is the very high per-iteration cost due to sparsity of the intermediate matrices. However, fast estimation of multinomial logit models that efficiently take advantage of the matrix structures have been proposed \[10\]. It overshoots the purpose of ABN as it requires tailored parametrisation. An alternative approach to estimate multinomial logistic regressions is to approximate it using multiple sequential binary logistic regressions. The primary purpose of the scoring procedure is to estimate goodness-of-fit metrics, then special care should be taken to compute the log-likelihood as each observations are counted multiple times. This estimation step substantially slows down the estimation process. A robust, easy to implement and fast solution to estimate unregularized multinomial regression models is to use neural networks with no hidden layers, no bias nodes and a softmax output layer. The optimisation is done through maximum conditional likelihood. This procedure is implemented in R by the nnet package \[29\].

2.2 Information theoretic scores

The implemented scores in ABN are AIC, BIC and MDL:

\[
AIC(A_s, D) = - \log P(D|\hat{\Theta}, A_s) + 2d, \tag{1}
\]

\[
BIC(A_s, D) = - \log P(D|\hat{\Theta}, A_s) + d/2 \log n, \tag{2}
\]

\[
MDL(A_s, D) = - \log P(D|\hat{\Theta}, A_s) + d/2 \log n + C_k, \tag{3}
\]

where \(\hat{\Theta}\) is the maximum likelihood parameters for \(A_s\) and \(P(D|\hat{\Theta}, A_s)\) is the maximum value of the likelihood function, \(d\) is the number of free
parameter, \( n \) is the sample size, \( k \) is the number of variables and 
\[ C_k = \sum_{j=1}^{k} (1 + |Pa_j|) \log k. \]

\(|Pa_j|\) is the size of the parent set of variable \( j \). Then the MDL is the BIC with an extra penalty for model complexity.

### 3 Software implementation

An ABN analysis is done using successive application of three functions.

```r
bsc.compute <- buildscorecache.mle(data.df = df.abn.,
 data.dists = dist, max.parents = 5)
dag <- mostprobable(score.cache = bsc.compute, score = "bic")
fit.dag <- fitabn.mle(dag.m = dag, data.df = bsc.compute$data.df,
 data.dists = dist)
```

In the R package ABN the `buildscorecache.mle()` function is essentially a wrapper of the `fitabn.mle()` function. It requires minimally: a named dataset, the named list of the distribution of the entries of the dataset and an upper limit for network complexity. It computes firstly an empty list of valid parent combination, using banning and retaining input matrices (which are assumed to be empty by default). Then it iterates through the cache to score the candidate piece of network. At each step of the scoring the used IRLS algorithm depends on the given list of distributions. For the special case of the binomial nodes, the usual logistic regression is tried, if it fails to estimate the given problem, a bias-reduced tailored algorithm is used. If however the algorithm fails to return a finite estimate, some predictors are sequentially removed until the design matrix becomes fully ranked. These three steps ensure ABN to be able to score a dataset even if it is data separated. In this example, an exact search algorithm is used to select the maximum a posteriori DAG (`mostprobable()`) Koivisto and Sood [13].

The `fitabn.mle()` function scores a given network. It requires a valid DAG, a named datasets and a named list of distributions. It returns the list of score for each node, the parameter estimates, the standard deviation and the \( p \)-values. Special care should be taken when interpreting and displaying the \( p \)-values. Indeed, the DAG has been selected using goodness of fit metric so adjustment methods should at least be used.

The Bayesian equivalent functions in ABN are `fitabn()` and `buildscorecorecache()`. Those function estimate Bayesian regression using following parameter priors: weekly informative Gaussian priors with mean zero and variance 1000
for each of the regression parameters of the model (both binomial and Gaussian), as well as diffuse Gamma priors (with shape and scale equal to 0.001) for the precision parameters in Gaussian nodes in the model.

### 3.1 Benchmarking

In order to benchmark the performances of the different possible implementations, complex BNs of 10 purely continuous nodes have been simulated. Then a dataset of 10'000 observations have been simulated from each BN. The benchmarking is performed based on 50 repetitions [20]. The different algorithms are:

1. fitabn: is the fitting procedure based on a tailored INLA code written in C (available in abn) [16];

2. glm.irls.cpp: is the Rcpp implementation of the IRLS algorithm (described in this article);

3. glm.irls.qrnewton: is an R implementation of the IRLS algorithm based on a QR decomposition in a Newton scheme;

4. glm.irls: is the R implementation of the IRLS algorithm [23];

5. glm.speedglm.wfit: is the R function `speedglm.wfit()` well adapted for matrix from SPEEDGLM in an switch scheme [4];

6. glm.speedglm: is the R function `speedglm()` from SPEEDGLM in a switch scheme [4];

7. glm.switch: is the R function `glm()` from STATS in a switch scheme [23].

As one can see in Figure 1, the Rcpp implementation (glm.irls.cpp) is the fastest which was one of the motivations of this project. However, the comparison is somewhat unfair as the different functions do not return the same output.

### 4 Simulation studies

In order to assess the performance of the ABN implementation a simulation study have been performed. The parameter which are important from a
Figure 1: Benchmarking comparison between different algorithm implementations to estimate regression coefficient in an abn framework on a logarithmic scale.

Simulation point of view are: the BN dimension (i.e. the number of nodes of the BN), the structure density (i.e. average number of parent per node) and the sample size. Additionally to those structure-wise metrics important factors impacting simulations are the intensity of the arc link, the variability of the arcs distributions and the mixture of variables. Indeed, scores used are only approximately score independent and increases in mixing distribution. Simulating randomly DAG structures are done through the simulation of adjacency matrices with constrains for ensuring acyclicity. Simulating observations from a given structure is done with random number generator in respecting the node ordering using JAGS [22].
4.1 Regression coefficients estimation

The Bayesian and MLE implementation are compared for parameter estimation accuracy in Figure 2. Two network densities, 20% and 80% of the possible arcs expressed, have been simulated 50 times. Then the regression coefficients have been computed for different sample size and the coefficient of variation of the given node as a proxy for distribution variability.

![Low density BN: Bayesian estimation](image1)

![Low density BN: MLE estimation](image2)

![High density BN: Bayesian estimation](image3)

![High density BN: MLE estimation](image4)

Figure 2: Comparison between Bayesian and MLE implementation to estimate regression coefficient in an ABN framework. The panels show the maximum Root Mean Squared Error (max RMSE) in function of the network density, the distribution variability and the sample size.

As one can see in Figure 2, the error measured as the maximum root mean squared error (max RMSE) on a log-log scale, both implementations produce very similar results. Even if the estimation frameworks are very different.
4.2 Score efficiency comparison

In order to estimate the efficiency of the different scores implemented in ABN, BNs with a given arc density have been simulated. Form those networks 20 datasets have been simulated for different sample sizes. The metrics used to display performance of the score are: the true positive (number of arc retrieved), false positive (learning an arc where there is not) and false negative (learning no arc where there is one). The scores used are abn (marginal posterior likelihood in a Bayesian regression framework), mlik (maximum likelihood) AIC, BIC and MDL.

As one can see in Figure 3 the mlik (maximum likelihood) is a suboptimal score for BN learning as expected by Daly et al. [3]. Indeed it tends to return fully connected BN. The Bayesian score (abn) seems to be the most efficient especially when the sample size is low. This score seems to be especially better at identifying the absence of arcs compared to other scores. The AIC seems to perform less effectively than the other information-theoretic scores due to its larger variability.
Figure 3: Score efficiency comparison for abn (marginal posterior likelihood), mlik (maximum likelihood), AIC, BIC and MDL for a given BN density in function of the number of observations using true positive, false positive and false negative metrics.
References

[1] Remco R Bouckaert. Bayesian network classifiers in weka for version 3-5-7. *Artificial Intelligence Tools*, 11(3):369–387, 2008.

[2] Denis Cornet, Jorge Sierra, Régis Tournebize, Benoît Gabrielle, and Fraser I Lewis. Bayesian network modeling of early growth stages explains yam interplant yield variability and allows for agronomic improvements in West Africa. *European journal of agronomy*, 75:80–88, 2016.

[3] Rónán Daly, Qiang Shen, and Stuart Aitken. Learning Bayesian networks: approaches and issues. *The knowledge engineering review*, 26(2):99–157, 2011.

[4] Marco Enea. *speedglm: Fitting Linear and Generalized Linear Models to Large Data Sets*, 2017. URL https://CRAN.R-project.org/package=speedglm. R package version 0.3-2.

[5] Julian J Faraway. *Extending the linear model with R: generalized linear, mixed effects and nonparametric regression models*, volume 124. CRC press, 2016.

[6] Simon M Firestone, Fraser I Lewis, Kathrin Schemann, Michael P Ward, Jenny-Ann LML Toribio, Melanie R Taylor, and Navneet K Dhand. Applying Bayesian network modelling to understand the links between on-farm biosecurity practice during the 2007 equine influenza outbreak and horse managers’ perceptions of a subsequent outbreak. *Preventive veterinary medicine*, 116(3):243–251, 2014.

[7] David Firth. Bias reduction of maximum likelihood estimates. *Biometrika*, 80(1):27–38, 1993.

[8] Andrew Gelman, Aleks Jakulin, Maria Grazia Pittau, Yu-Sung Su, et al. A weakly informative default prior distribution for logistic and other regression models. *The Annals of Applied Statistics*, 2(4):1360–1383, 2008.

[9] Joseph F Hair, William C Black, Barry J Babin, Rolph E Anderson, Ronald L Tatham, et al. *Multivariate data analysis*, volume 5. Prentice hall Upper Saddle River, NJ, 1998.
[10] Asad Hasan, Zhiyu Wang, and Alireza S. Mahani. Fast estimation of multinomial logit models: R package mnlogit. *Journal of Statistical Software*, 75(3):1–24, 2016. doi: 10.18637/jss.v075.i03.

[11] David Heckerman, Dan Geiger, and David M Chickering. Learning Bayesian networks: The combination of knowledge and statistical data. *Machine learning*, 20(3):197–243, 1995.

[12] Markus Kalisch, Martin Mächler, Diego Colombo, Marloes H. Maathuis, and Peter Bühlmann. Causal inference using graphical models with the R package pcalg. *Journal of Statistical Software*, 47(11):1–26, 2012. URL http://www.jstatsoft.org/v47/i11/.

[13] Mikko Koivisto and Kismat Sood. Exact Bayesian structure discovery in Bayesian networks. *Journal of Machine Learning Research*, 5(May):549–573, 2004.

[14] Ioannis Kosmidis and David Firth. Bias reduction in exponential family nonlinear models. *Biometrika*, 96(4):793–804, 2009.

[15] Gilles Kratzer, Marta Pittavino, Fraser Lewis, and Reinhard Furrer. abn: an R package for modelling multivariate data using additive Bayesian networks. *R package vignette*, 2017.

[16] Fraser I Lewis and Michael P Ward. Improving epidemiologic data analyses through multivariate regression modelling. *Emerging themes in epidemiology*, 10(1):4, 2013.

[17] Antoinette Ludwig, Philippe Berthiaume, Patrick Boerlin, Sheryl Gow, David Léger, and Fraser I Lewis. Identifying associations in Escherichia coli antimicrobial resistance patterns using additive Bayesian networks. *Preventive veterinary medicine*, 110(1):64–75, 2013.

[18] BJ McCormick. Frequent symptomatic or asymptomatic infections may have long-term consequences on growth and cognitive development. In *Old Herborn University Seminar Monographs*, pages 23–39. Institute for Microbiology und Biochemistry Herborn, Germany, 2014.

[19] BJJ McCormick, MJ Sanchez-Vazquez, and FI Lewis. Using Bayesian networks to explore the role of weather as a potential determinant of disease in pigs. *Preventive veterinary medicine*, 110(1):54–63, 2013.
[20] Olaf Mersmann. *microbenchmark: Accurate Timing Functions*, 2018. URL https://CRAN.R-project.org/package=microbenchmark. R package version 1.4-4.

[21] Kevin Murphy et al. The Bayes net toolbox for Matlab. *Computing science and statistics*, 33(2):1024–1034, 2001.

[22] Martyn Plummer et al. JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. In *Proceedings of the 3rd international workshop on distributed statistical computing*, volume 124. Vienna, Austria, 2003.

[23] R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2017. URL https://www.R-project.org/.

[24] Robert W Robinson. Counting unlabeled acyclic digraphs. In *Combinatorial mathematics V*, pages 28–43. Springer, 1977.

[25] Sabrina Ruchti, Andrea R. Meier, Hanno Würbel, Gilles Kratzer, Sabine G. Gebhardt-Henrich, and Sonja Hartnack. Pododermatitis in group housed rabbit does in switzerland – prevalence, severity and risk factors. *Preventive Veterinary Medicine*, 2018. ISSN 0167-5877. doi: https://doi.org/10.1016/j.prevetmed.2018.06.011. URL http://www.sciencedirect.com/science/article/pii/S0167587718300813.

[26] Marco Scutari. Learning Bayesian networks with the bnlearn R package. *Journal of Statistical Software*, 35(3):1–22, 2010. doi: 10.18637/jss.v035.i03.

[27] Marco Scutari. Dirichlet Bayesian network scores and the maximum relative entropy principle. *Behaviorometrika*, pages 1–26, 2018.

[28] Peter Spirtes. An anytime algorithm for causal inference. In *AISTATS*, 2001.

[29] W. N. Venables and B. D. Ripley. *Modern Applied Statistics with S*. Springer, New York, fourth edition, 2002. URL http://www.stats.ox.ac.uk/pub/MASS4 ISBN 0-387-95457-0.
[30] Timothy C Wilcosky and Lloyd E Chambless. A comparison of direct adjustment and regression adjustment of epidemiologic measures. *Journal of chronic diseases*, 38(10):849–856, 1985.

[31] Christopher Zorn. A solution to separation in binary response models. *Political Analysis*, 13(2):157–170, 2005.

[32] Yuan Zou and Teemu Roos. On model selection, Bayesian networks, and the fisher information integral. *New Generation Computing*, 35(1):5–27, 2017.