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Bayesian Challenges in Integrated Catchment Modelling

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Abstract: Bayesian Networks (BNs) are increasingly being used as decision support tools to aid the management of the complex and uncertain domains of natural systems. They are particularly useful for addressing problems of natural resource management by complex data analysis and incorporation of expert knowledge. BNs are useful for clearly articulating both the assumptions and evidence behind the understanding of a problem, and approaches for managing a problem. For example they can effectively articulate the cause-effect relationships between human interventions and ecosystem functioning, which is a major difficulty faced by planners and environment managers. The flexible architecture and graphical representation make BNs attractive tools for integrated modelling. The robust statistical basis of BNs provides a mathematically coherent framework for model development, and explicitly represents the uncertainties in model predictions. However, there are also a number of challenges in their use. Examples include i) the need to express conditional probabilities in discrete form for analytical solution, which adds another layer of uncertainty; ii) belief updating in very large Bayesian networks; iii) difficulties associated with knowledge elicitation such as the range of questions to be answered by experts, especially for large networks; iv) the inability to incorporate feedback loops and v) inconsistency associated with incomplete training data. In this paper we discuss some of the key research problems associated with the use of BNs as decision-support tools for environmental management. We provide some real-life examples from a current project (Macro Ecological Model) dealing with the development of a BN-based decision support tool for Integrated Catchment Management to illustrate these challenges. We also discuss the pros and cons of some existing solutions. For example, belief updating in very large BNs cannot be effectively addressed by exact methods (NP hard problem), therefore approximate inference schemes may often be the only computationally feasible alternative. We will also discuss the discretisation problem for continuous variables, solutions to the problem of missing data, and the implementation of a knowledge elicitation framework.

Keywords: Bayesian networks; Integrated Catchment Management; Decision support for natural resource management.

1. INTRODUCTION

The European Water Framework Directive (WFD) sets out an integrated perspective to water management where the river catchment and river basin district are the scales of focus. It encourages the active involvement of all affected parties within the planning process [Giupponi, 2007]. At these large spatial scales, there are always competing and often conflicting management challenges that need to be addressed, such as demands for water of good quality, the integrity of aquatic ecosystems and flood risk management. In turn, the water related objectives must be pursued within the broader context of economic, social, cultural and other environmental objectives for the catchment as a whole. Given these challenges, decision making must be supported by new tools which evaluate the potential impacts of planned management interventions on multiple objectives.

These new tools are often equated with integrative models. Integrative models are typically developed for five main reasons: i) prediction; ii) forecasting; iii) management and decision making; iv) social learning; v) developing system understanding and experimentation. The types of models suited to integrated catchment management include system dynamics, Bayesian networks, metamodels, coupled complex models, agent based models and expert systems. In this paper we focus on Bayesian networks.

Bayesian networks provide a useful tool to assist in the structuring and analysis of decision problems [Watthayu and Peng, 2004]. A Bayesian network is a decision analysis framework, based on Bayesian probability theory, which allows the integration of scientific and experiential knowledge, and the uncertainty associated with this knowledge [Castelletti and Soncini-Sessa, 2007]. The approach involves describing a system in terms of variables and linkages, or relationships between variables, at a level appropriate to the decision making. This is achieved through representing linkages as conditional probability tables and propagating probabilities through the network to give the likelihood of variable outcomes [Murphy, 2001]. Therefore, the approach ensures that the treatment of risks and uncertainties is an intrinsic part of the decision-making processes [Borsuk et al., 2004]. The Bayesian network is flexible and interactive, and hence if a previously developed network does not fit a user's conceptual understanding of the system, it can be adapted quickly and simply to the cognitive understanding of the user.

The scope and feasibility of BNs in integrated catchment modelling are currently being investigated by the Catchment Science Centre (CSC) at the University of Sheffield. The model, termed the Macro-Ecological Model (MEM), is being designed to model the links between the technical, economic and social processes which interact within any given catchment. The aim is to develop a decision support tool, combining a simulation model of the causal relationships within catchment processes with plausible scenarios of management options. The tool will estimate a set of indicators which stakeholders can use to inform their decisions. In this paper we discuss some of the challenges of BNs in developing this model.

2. BN CHALLENGES IN INTEGRATED CATCHMENT MODELLING

2.1 Building large networks

Developing an integrated catchment model like the MEM involves many components which, when translated into a BN become a large network. From a practitioners' point of view, the process of compiling and executing a BN, using the latest software tools and improved computational power, is relatively easy. Also, the accuracy and speed of current algorithms makes it feasible for an application in integrated catchment management. However, the problems of building a complete BN for a particular "large" problem remain a complex task. Designing the right network structure is a prerequisite for meaningful elicitation of any probabilities. It needs proper software and knowledge engineering practice during the development phase. Knowledge engineers work with experts to decompose the system, recognise patterns at the macro and micro level [Shaw and Garland, 1996] and continually change the model as both sides' understanding increases. The

benefits of constructing software systems from components or modules are well known and the properties that modular systems must contain were articulated as early as 1972 [Parnas, 1972]. However, little work has been done on applying modular structures in BN design. Laskey and Mahoney recognised that BN construction required a method for specifying knowledge in larger, semantically meaningful, units they called network "fragments" [Laskey and Mahoney, 1997]. Laskey and Mahoney also argued that current approaches lacked a means of constructing BNs from components. The available development software for BNs lack sophisticated software engineering tools compared to the modern software development tools available for the mainstream software industry where these forms parts of an integrated development environment. In the MEM project, we follow a "bottom up" approach decomposing the model into fragmented modules that, when joined together, form the complete system. A fragmented module, which we call a sub-network, is a set of related system variables that could be constructed and reasoned about separately from other sub-networks. However consistency must be maintained in defining the common variables across different sub-networks. Ideally, sub-networks must make sense to the expert who must be able to supply some underlying motive or reason for the variables belonging together. In Figure 1 a simplified subset of the MEM network has been depicted showing how the developed sub-networks are linked together. The focus in Figure 1 is on the 'connector' variables of "PO_4 concentration" and "River discharge" that enable the different sub-networks to be connected. Another approach could be to use an object-oriented methodology where fragmented modules become classes, both variables (nodes) and instantiated BN fragments become objects and encapsulation is implemented via an interface and private variables [Koller and Pfeffer, 1997]. Connector variables can be used to specify interfaces and intermediate variables can encapsulate private data. However this can be difficult to follow strictly because different sub-networks can contain the same connector node as an intermediate variable. When creating an object of a sub-network we must know whether it shares intermediate nodes with other sub-network objects in order to define the influence combination rule. Clearly this is not a problem when the influence combination rule treats all parent nodes equally irrespective of type and value, as a form of dynamic polymorphism, but such a combination rule would be very difficult to conceive and implement [Neil et al., 2000].
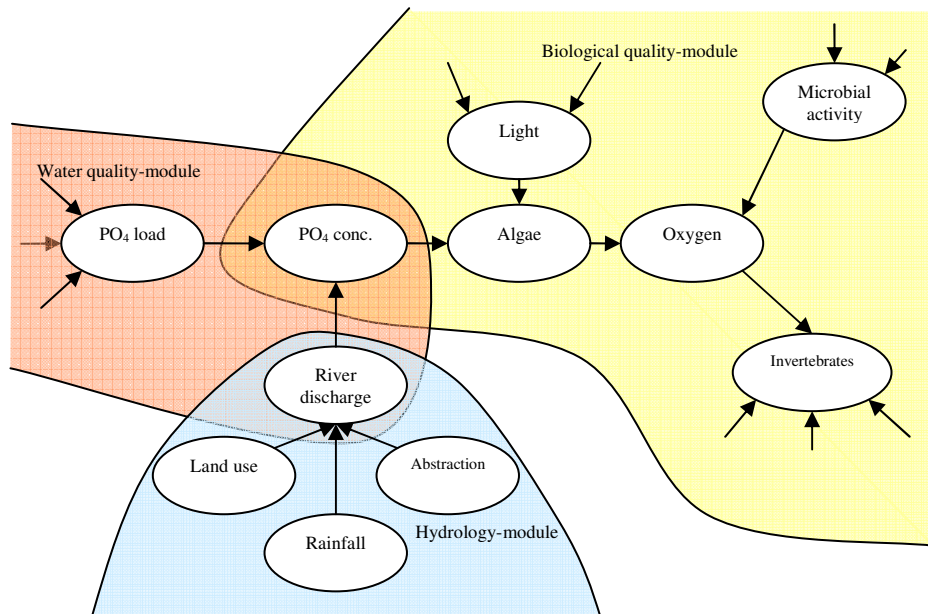

Figure 1. Subset of the MEM network showing how the developed sub-networks are linked together

2.2 Inventing hidden node

One of the major steps in large domain modelling is structural simplification. Such simplification is necessary for greater compactness and to reduce the computational complexity. A more interesting problem is inventing hidden nodes. Hidden nodes can make a model much more compact (see Figure 2). Introducing hidden nodes to the network structure may reduce the computational complexity of a Bayesian network by reducing its dimensionality, and may also help to capture non-trivial (higher order) correlations between observed events. However hidden nodes may also be included in a Bayesian network structure to reflect expert domain knowledge regarding hidden causes and functionalities which impose some structure on the interaction among the observed variables.
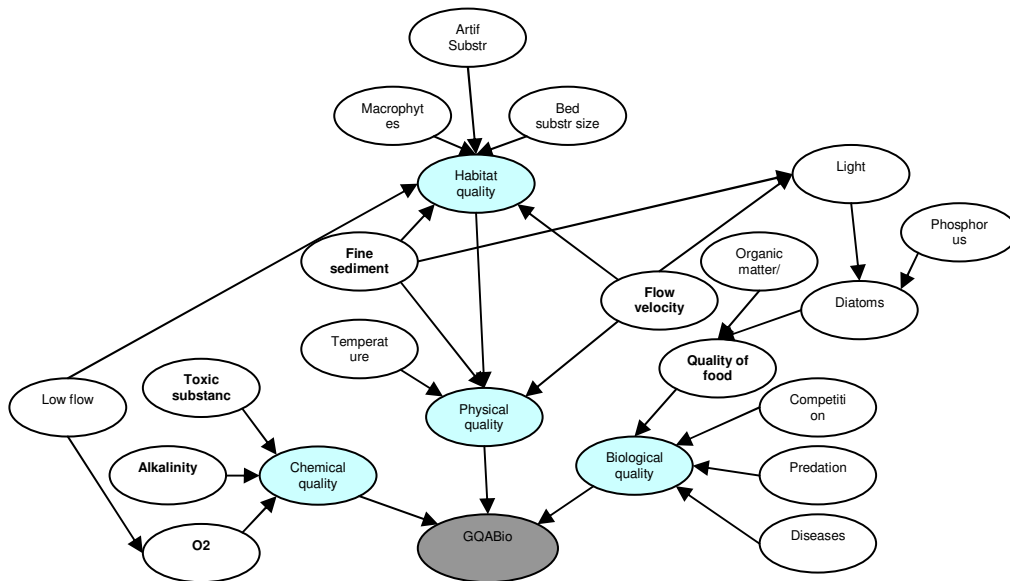

Figure 2. Conceptual biological quality network where light blue bubbles represent hidden nodes, white bubbles represent observed variables and the grey bubble represents the index variable (GQABio = General Quality Assessment score for Biology).

Generally hidden nodes should be added in consultation with experts or they should be added during structural learning. One problem is choosing the cardinality (number of possible values) for the hidden node, and its type of Conditional Probability Distribution. Another problem is choosing where to add the new hidden node. There is no point making it a child, since hidden children can always be marginalized away, so we need to find an existing node which needs a new parent, when the current set of possible parents is not adequate [Heckerman, 1995]. Furthermore, interpreting the "meaning" of hidden nodes is always tricky, especially since they are often unidentifiable. One way is to follow fully automated structure discovery techniques which can be useful as hypothesis generators and which can then be tested by experiment. In the MEM the simplification process has been done in consultation with domain experts and hidden nodes are generally some proxy indices used by the Environment Agency.

2.3 Learning with distributed datasets

Training datasets have been classified as fully observable (which means that the values of all variables are known) and partially observable (meaning that we do not know the values of some of the variables) [Heckerman, 1995]. Partial observability might occur because variables are measured at different spatial points (we call this a distributed dataset), through a change in survey strategy (introducing or excluding some of the variables), due to missing

records for certain observation (called missing variables), or simply because certain variables cannot be measured (hidden variables). Learning approaches from partial observability are confined to dealing with the issue of missing values. When some variables are missing, the likelihood surface becomes multimodal. The problem of simple missing values in the dataset has been addressed very simply in Bayesian networks, because likelihoods can be computed using normal iterative methods (such as gradient decent or Expectation-Maximization (EM)) [Heckerman, 1995]. These iterative methods try to find a local maximum of the Maximum Likelihood (ML) or Maximum A Posterori (MAP) function [Murphy, 2001]. This capability of BNs has been cited as very useful as there is no minimum data requirement to perform the analysis and BNs take into account all the data available [Myllymaki et al., 2002]. However, there are many practical cases where the observed dataset is distributed among different sites which make a distributed heterogeneous dataset scenario, where each site has observations corresponding to a subset of the attributes. In some cases we have only a small set of overlapping data points from which it is not sufficient to derive casual relationships. It will be difficult or impossible (depending on the scenarios) to find local maxima in the ML/MAP function for such distributed datasets. Iterative algorithms need to use an inference algorithm to compute the expected sufficient statistics which will be difficult for an extreme missing value problem. So learning from distributed datasets is not possible with conventional learning methods.

In the MEM project we have tried to tackle this problem using an Artificial Neural Network (ANN) approach. The goal was to build a constant predictor by using distributed datasets. Different ANN predictors were built mapping subsets of predictor variables with response variables which are combined into a single model over a weighted average. The weights are determined by training based on the small overlapping dataset and they represent the prediction capability of each sub-model.

2.4 Discretisation of continuous variables

A large number of the observation data required for the development of the MEM are continuous data (e.g. phosphate concentration). Bayesian networks can deal with continuous variables in only a limited manner. If continuous variables are to be incorporated in BNs some means must be found of *optimally* partitioning the values into sub-ranges which can then be treated as discrete categories. The way this discretisation is performed affects the performance of the subsequently derived BN model.

In order to maximise the predictive power of BNs, it is necessary to discretise each of the continuous input variables in some optimal manner. Every continuous variable could require differing numbers of bins which might well also be of non-uniform width. The problem is thus one of identifying the optimal set of binning parameters. Genetic algorithms (GAs) have proved very successful at solving this sort of discrete search problem and we propose employing them here. GAs work by evolving a population of possible solutions in a manner analogous to Darwinian survival of the fittest. For N continuous input variables to the BN, we require some set of bin widths spanning each variable's range. The number of bins and their widths can differ between and indeed within variables. We propose constructing a GA individual (a chromosome) as a set of N lists of binning schedules, one list per BN input variable. At each iteration of the GA, stochastically-selected pairs of individuals will be crossed-over and mutated using specially adapted genetic operators; the objective function 'driving' the evolution will be the predictive power of a BN employing the binning schedule specified by a given chromosome. In this way, the set of bin specifications yielding the (near-) optimal performance will be generated. We envisage significantly improved predictive power for BNs. Figure 3 shows some results of this exercise where we show performance comparison of a GA approach with the classical 1R method proposed by Holte et al. [1989]. There is a marked increase in predictability of the target variable with the GA approach. The technique should also be applicable to decision trees which are a very widely used learning paradigm operating on nominal variables.
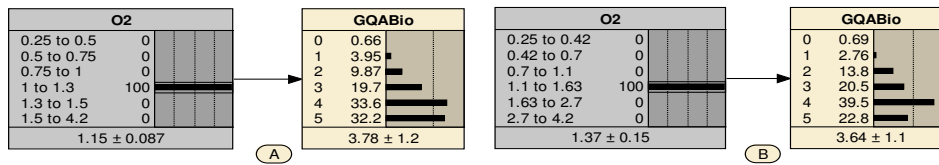
O2		GQABio	
0.25 to 0.5	0	0	0.66
0.5 to 0.75	0	1	3.95
0.75 to 1	0	2	9.87
1 to 1.3	100	3	19.7
1.3 to 1.5	0	4	33.6
1.5 to 4.2	0	5	32.2
1.15 ± 0.087		3.78 ± 1.2	

O2		GQABio	
0.25 to 0.42	0	0	0.69
0.42 to 0.7	0	1	2.76
0.7 to 1.1	0	2	13.8
1.1 to 1.63	100	3	20.5
1.63 to 2.7	0	4	39.5
2.7 to 4.2	0	5	22.8
1.37 ± 0.15		3.64 ± 1.1	

Figure 3. Performance of discretisation algorithms: (A) 1R method [Holte et al., 1989]; (B) Optimization using Genetic algorithm.

2.5 Expert knowledge elicitation and structuring

Bayesian networks allow for casual relationship (probabilities) to be specified based on subjective assessments ("expert opinion"), empirical evidence, or a combination of both. Incorporating expert opinion is important because, often, there are insufficient data to learn and model relationships between casual factors and outcomes using population-based data ("machine learning"). When there is a paucity of data, domain expert opinion can be used to create Bayesian networks. Expert-derived probabilities can be improved over time with observational data from multiple sources, obviating the need for a single data repository that contains all casual relationships. However the number of probability distribution required to populate a Conditional Probability Table (CPT) grows exponentially with the number of parent nodes. The sheer volume of questions to be answered by the experts poses a considerable cognitive barrier. Also extracting knowledge in a form that can be converted into probability distributions may prove difficult in real life situations. This is because many field experts are used to working with real sampling or experimental data, and may find it difficult to provide any numbers without relying on data. Also they may be used to classical statistical analyses and feel uncertain when trying to think about their knowledge in terms of probability distributions rather than point estimates and confidence intervals. This uncertainty together with only superficial knowledge about the methodology may also lead to distrust towards the BNs, which easily leads to reluctance to provide the estimates.

Some well-known methods in this area are the Noisy-OR model [Pearl, 1998] and some improvement and generalisation by others [Henrion, 1989; Srinivas, 1993]. These models can compute the distributions needed for the CPT from a small set of questions elicited from the expert. All these models, however, are constrained by the assumption that parents act independently without synergy [Srinivas, 1993].

For the MEM project we are implementing a modified version of the relative weight and compatible probability method proposed by [Das, 2004]. The input to the algorithm consists of a set of weights that quantify the relative strengths of the influences of the parent nodes on the child node and a set of compatible probability distributions. The number of questions grows linearly with the associated parent nodes. We introduced a special case when certain parent nodes are critical and have some thresholds, above or below which the effect of other parent nodes is none or minimal. For example in the biological quality network shown in Figure 4, oxygen can be a critical variable. We asked a few more questions to the experts to elicit the critical variables and their critical states. The same set of questions has also been used for cross validation and intra consistency check of expert knowledge. Figure 4 shows a simple outcome comparing results from the original approach of Das with those from the modified approach we have used in the MEM project. Because the variable 'oxygen' is a critical variable under approach B, its existence in a low state has a far stronger influence on the outcome of GQABio than under approach A where oxygen has not been identified as a critical variable.
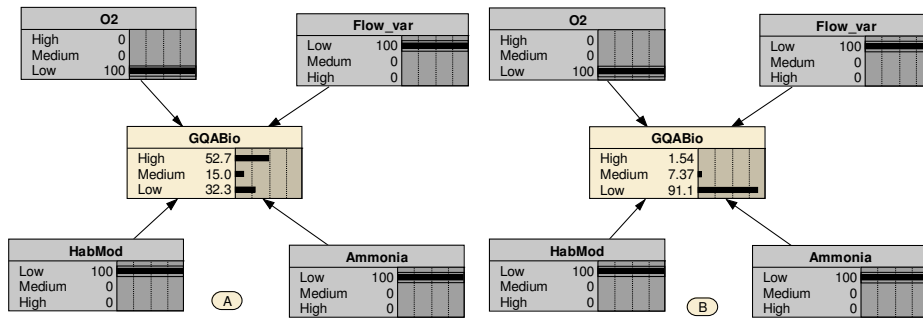
Figure 4. Results for a critical case (Oxygen low) (A) implemented with [Das, 2004] knowledge elicitation approach (B) Modified version of [Das, 2004] developed for MEM.

2.6 Dynamic model structure and feedback loops

BNs are static models and as such not able to integrate system dynamics and feedback loops. However, there are different ways of dealing with this issue when applying BNs for modelling dynamic systems. The simplest approach is to assume that the system under consideration is in equilibrium. For example in the MEM sub-network of water quality, phosphate concentration in the river has been taken as annual mean PO_4 concentration. A more sophisticated approach to incorporate temporal and ambient aspects is the Dynamic Bayesian Network (DBN) approach. The predominant DBN literature [Korb and Nicholson, 2004; Murphy, 2002] deals with contiguous time slice models based on the Markov assumption that the current state of the model depends on its previous time state and action taken in its current state. However a known impediment of this approach is the exponential increase in network size apart from the knowledge acquisition problem. Figure 5 shows a simple two-node feedback loop for 3 time steps (A0-A3 and B0-B3). Many solutions are being proposed to solve feedback loops in DBNs but most of them still need to be tested in practical applications. For example, Gossink et al. [2007] have proposed an extended version of DBN to ease the "intractability of knowledge acquisition" problem. The inference algorithm used for this approach is likelihood weighted approximation. Exact algorithms are still not applied with this approach and modification of the extended DBN may be needed [Gossink et al., 2007].

Even if we decided to build a time sliced DBN, inference is another problem at a later stage. It needs to unroll the network to represent dependencies between nodes from two consecutive time slices. Further, it needs to preserve conditional relationships between nodes as well as influence that evidence nodes have on hidden nodes (if there are any). Parameter learning can be difficult and the main reason is unquantified uncertainty in the elicited

Figure 5. Dynamic Bayesian Network representing a feedback loop.

probabilities. Further, a dynamic network can have a static node which creates a problem of dependency and representation. [Schafer and Weyrath, 1997] claimed that the problems in this type of model can be differentiated in two classes: (a) the dependency between dynamic child node and static parent node, and (b) the initial value of static node is not known with certainty, and we can only estimate this node's value which could be changed as time progresses. Schafer and Weyrath claimed that the dependency can be interpreted by incorporating the effect of the static node in the dynamic node, so the dynamic node will
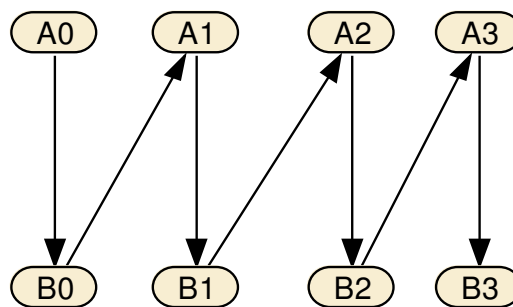
convey all of the information needed for inference. Problem (b) can be solved if we compromise accuracy for efficiency in a way that can delay rollup until we receive the exact probability of the static node.

2.7 Belief updating

BNs for a large domain like ICM are implemented as a modular network consisting of many subnets joined together to form the complete system. Consistency among subnets in an integrated BN is achieved by communication. When a subnet updates its belief, it communicates with an adjacent subnet to maintain the consistency across the system. Large-scale models generally have high-order stochastic dependencies. The computational complexity of treating these dependencies exactly can be characterized in terms of the size of the maximal clique of the "moralized" graph [Murphy, 2002]. Existing inference algorithms [Xiang, 1995] require repeated belief propagations (which is proportional to the number of linkages between the subnets) within the receiving subnet. It has been stated that singly connected BNs are tractable and have time algorithm linear in the number of nodes in a network or the size of the network for exact inference [Cooper, 1990]. On the other hand, multiply connected Bayesian networks are intractable and do not admit efficient algorithms for exact inference in the worst case which makes the exact inference in BNs to be NP-hard [Cooper, 1990]. Others [Murphy, 2002; Xiang, 2000] believe that inference in a BN can be performed effectively using its junction tree (JT) representation. However, the junction tree propagation method cannot compute $p(X|e)$ when X is not contained in a node of the junction tree. Also, the local propagation procedure has to be applied whenever new evidence is observed. [Xiang, 2000] has worked on extending junction trees beyond single BNs and tried to prove that two local propagations are sufficient for propagating evidence from one JT to an adjacent one no matter how many linkages there are between the two JTs. This results in big computational savings which are particularly significant for a large domain with subnets comprising multiple linkage JTs.

The complexity of the exact inference algorithm does not mean that we cannot solve inference in large BNs. It implies that we cannot find a general procedure that works for all networks. However, depending on the network complexities, we can have an efficient algorithm either exact or approximate. Various algorithms e.g. approximate, heuristic, hybrid or special case algorithms should be taken into consideration for a large domain network. A future research goal should be that of identifying effective approximate algorithms that work well for large domain problems. Also the integration of various kinds of exact and approximate algorithms exploiting the best of each can be an interesting area of research.

There are other problems which we have not discussed in this paper but which are relevant for ICM modelling. In the missing value problem there is a particular case reported by [Rubin, 1978]: failure to observe a variable may in itself be informative about the true state of the system. For example, in habitat survey data, failure to report a population of a certain species may suggest that system state is not suitable for survival of that species. In medical science, researchers have worked on this problem and proposed methods for dealing with such situations [Chickering and Pearl, 1996; Robins, 1986; Rubin, 1978].

3. CONCLUSION

Bayesian networks are still a relatively new approach but they are gaining popularity in many application areas, including environmental applications. Many easy-to-use BN development software packages are available but they are still lacking the sophistication and robustness of a standard development environment. Also they are not updated with the ongoing developments in the field of BN research. Integrated Catchment Management modelling provides its own set of challenges to BNs. Questions that need to be addressed in the context of applying BNs for ICM are: Do we have data of sufficient quantity and quality? Is expert knowledge sufficient for model characterisation? Which algorithm should we use for inference, in order to extract valuable information and keep the computational complexity low? There are number of promising research avenues, challenges, and needs

that directly concern the usefulness of Bayesian networks and their impact on real world environmental applications.

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