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A comparison of two sensitivity analysis techniques based on four bayesian models representing ecosystem services provision in the Argentine Pampas



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ABSTRACT

Sensitivity analyses (SAs) identify how an output variable of a model is modified by changes in the input variables. These analyses are a good way for assessing the performance of probabilistic models, like Bayesian Networks (BN). However, there are several commonly used SAs in BN literature, and formal comparisons about their outcomes are scarce. We used four previously developed BNs which represent ecosystem services provision in Pampean agroecosystems (Argentina) in order to test two local sensitivity approaches widely used. These SAs were: 1) One-at-a-time, used in BNs but more commonly in linear modelling; and 2) Sensitivity to findings, specific to BN modelling. Results showed that both analyses provided an adequate overview of BN behaviour. Furthermore, analyses produced a similar influence ranking of input variables over each output variable. Even though their interchangeably application could be an alternative in our bayesian models, we believe that OAT is the suitable one to implement here because of its capacity to demonstrate the relation (positive or negative) between input and output variables. In summary, we provided insights about two sensitivity techniques in BNs based on a case study which may be useful for ecological modellers.

1. Introduction

Bayesian Networks (BN) consist on a set of variables with a probabilistic distribution, and their outcome assesses how likely events are and how these probabilities change with external interventions (Jensen and Nielsen, 2007; Korb and Nicholson, 2004). A BN can be represented visually as a set of nodes connected by direct links (Fig. 1). Nodes represent variables and the probability distribution of their possible states, while links represent causal relationships between nodes (Kristensen and Rasmussen, 2002). Nodes with no incoming arrows are parent nodes (i.e. input variables); while nodes with incoming arrows are child nodes (i.e. parameters) (McCann et al., 2006). Each node can take different states (e.g. high/medium/low) which are clusters delimited by intervals or ranges (Fig. 1). The number of states is dependent on the information conveyed and the possible values that they can get (Dlamini, 2010). Parent nodes have marginal probabilistic distributions that represent the frequency of each state, while child nodes are characterized by a conditional probability table that represents a factorial combination of its parent nodes along with their probabilistic values (Chen and Pollino, 2012).

Currently, BNs are an increasingly accepted method for modelling uncertain and complex domains, such as ecosystems (Uusitalo, 2007). The conceptual representation of BN results (i.e. graphical networks) is very useful for an intuitive presentation of functional relationships within complex systems. Their advantages are commonly related to the flexibility for dealing with both expert knowledge and system uncertainty (Borsuk et al., 2004; Castelletti and Soncini-Sessa, 2007). BNs have been used for modelling in a wide range of disciplines like psychology (López Puga et al., 2007), education (García et al., 2007), ecological risk assessment (Pollino et al., 2007), agroecosystems sustainability (Ticehurst et al., 2007) and ecosystem services provision (Rositano and Ferraro, 2014), among others. Regarding natural resource management, BNs are able to both capture the influence of management decisions on key ecological variables, and to help decision makers on selecting the best course of action (McCann et al., 2006).

As in other modelling methodologies, BNs require the assessment of their performance. Validation is "a demonstration that a model within its domain of applicability has a satisfactory range of accuracy consistent with the intended application of the model" (Rykiel, 1996). Model validation is not an easy process and, as a consequence, should

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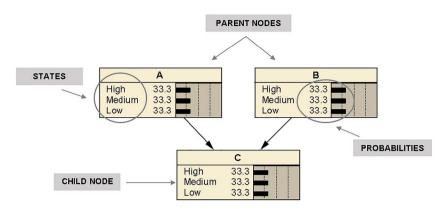


Fig. 1. Example of a Bayesian Network with three variables or nodes (A, B and C). Nodes A and B are parent nodes, while node C is a child node. Each node has three states (High, Medium and Low) with a uniform probability distribution.

be done with multiple strategies (Bert et al., 2014). Rykiel (1996) stated that sensitivity analyses (SAs) could be considered a strategy of model validation. Results of SAs are able to highlight the critical aspects of model development and data collection by identifying the impact of a change in input variables over the output variable (Newham et al., 2003; Thogmartin, 2010). Two groups of SAs are recognized: local and global (Saltelli et al., 2000). In local SA, parameter values are changed one at a time, while fixing all other variables. These SAs are not able to capture potential interactions among input variables as well as they partially explore parametric aspects (Cariboni et al., 2007; Hu et al., 2015; Saltelli and Annoni, 2010). Global SA involves varying all or several input variables at the same time, thus allowing identification of non-linear interactions among parameters (Confalonieri et al., 2010; Mackler-Pick et al., 2011). Lee et al. (2015) describe many techniques to carry out global SA. Taking this into account, environmental modellers need to be aware about the particularities of sensitivity methodologies in order to conduct a proper validation process (Cariboni et al., 2007).

Validating BNs is not simple to carry out (Payraudeau and van der Werf, 2005). In current practice, if a user has sufficient data on the phenomenon of interest, this data may be used to validate model predictions. However, BNs are commonly used to model complex systems with limited data (Chen and Pollino, 2012). Because of this, expert opinion could be an option to validate the structure, discretization and parameterization of bayesian models (Korb and Nicholson, 2004). Although expert test is quite simple, it is not sufficient to verify model validity in an independent way (Pitchforth and Mengersen, 2013). Aguilera et al. (2011) reviewed the use of BNs for environmental modelling and highlighted that ca. 40% of the studies showed no type of model validation, while only 13% of the models reviewed were validated through any kind of SA, like variance reduction (e.g. Marcot et al., 2006; Stelzenmüller et al., 2010), one-at-a-time (e.g. Bednarski et al., 2004; Chan and Darwiche, 2004; Coupé and van der Gaag, 2002; Coupé et al., 1999), sensitivity to findings (e.g. Chen and Pollino, 2012; Grêt-Regamey and Straub, 2006; Marcot, 2012; Pollino et al., 2007; Smith et al., 2007) or Latin hypercube sampling method (e.g. Borsuk et al., 2004). One-at-a-time (OAT) is the simplest methodology in order to obtain the effect of variation of parameter estimate on posterior probabilities (Coupé et al., 1999). Nonetheless, some authors have pointed out that this SA is not suitable for probabilistic methodologies (Chen and Pollino, 2012). A SA currently available in BN software packages, like Hugin (Madsen et al., 2005) or Netica (Norsys Software Corp., 2009), is "Sensitivity to findings" (STF) which is able to assess how much a finding at one variable will likely change the beliefs at another variable (Korb and Nicholson, 2004). It should be carried out with the BN previously populated since results change according to the quantitative information included into the model; therefore, this analysis is recalculated each time new information is collected. As well as OAT, this SA is only done to one variable at a time (Uusitalo, 2007). Despite conflicting opinions on which SA is the most appropriate

(Saltelli and Annoni, 2010), BN modellers should be aware about advantages and disadvantages when using each approach.

In BN literature, both kinds of SAs have been used to evaluate bayesian models; however, their comparison is lacking. A case study could be useful for doing a first attempt to highlight differences and similarities between these SAs. For that reason, we used previously developed BNs originally applied for assessing four ecosystem services provision (i.e. Soil Carbon balance, Soil Nitrogen balance, N₂O emission control, and Groundwater contamination control) in the Pampa region (Argentina) (Rositano and Ferraro, 2014). Therefore, the objective of this paper was to evaluate and compare the information provided by two local SAs: one used in BNs but more commonly in linear modelling (OAT), and one specific for BN modelling (STF).

2. Methodology

2.1. Bayesian models development

Ecosystem services (ES) offer the possibility to evaluate changes in ecosystems caused by human action and to resolve conflicts arised by different land uses (Vihervaara et al., 2010). In this sense, Rositano and Ferraro (2014) developed a framework to assess changes in ES provision as a consequence of environmental variability and agricultural management practices in Pampean agroecosystems (Argentina). The framework was based on two tools capable of dealing with ecosystems complexity and uncertainty: conceptual networks and probabilistic networks (i.e. BNs).

First, a conceptual network was developed representing the set of environmental and productive variables that determine the provision of eight ES in the Pampa Region. ES selected were: 1) Soil Carbon (C) balance, 2) Soil Nitrogen (N) balance, 3) Soil structure maintenance, 4) Soil water balance, 5) N₂O emission control, 6) Biotic adversities regulation, 7) Groundwater contamination control, and 8) Species richness maintenance. This list is based on an ES concept which not only includes the attributes and processes of those ecosystems that support ES, but also strictly services. The conceptual network was the result of a bibliographic review and an expert knowledge elicitation through semistructured interviews. Experts considered were researchers involved in several areas related to agroecosystems functioning (e.g. crop fertilization, contamination by fertilizers, nutrient dynamics, groundwater quality, soil fertility, weed ecophysiology). Researchers were selected within the academic field of Facultad de Agronomía, Universidad de Buenos Aires (FAUBA) as well as within other national universities and institutions. The expert panel was finally composed by 20 researchers.

Second, four sub-networks detached from the general conceptual network were selected in order to parameterize them with BNs. These sub-networks were: 1) Soil C balance, 2) Soil N balance, 3) N₂O emission control, and 4) Groundwater contamination control. The parameterization process consists on obtaining the conditional probabilities of child nodes (parameters) based on a conceptual network previously

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developed (Bressan et al., 2009). Prior to this process, it was necessary to determine the number of states (e.g. three states: high, medium, and low) of each node. In our case, nodes had between two and three states (see Appendix 1). Conditional probability tables were the result of a process of knowledge elicitation from a subset of those experts interviewed during the previous stage.

Finally, parent nodes (input variables) were quantified with environmental and productive databases from three agricultural areas in the Pampa region with different agro-ecological characteristics. Environmental databases were provided by the National Meteorological Service and the National Institute of Agricultural Technology, while productive databases were obtained from the Argentine Association of Regional Consortia of Agricultural Experimentation. Then, ES provision level was obtained for ten growing seasons (2000/2001–2009/2010) and three crops (wheat, maize and soybean).

2.2. Sensitivity analyses

Before quantifying input variables (parent nodes) with environmental and productive information, we needed to assess the performance of the four bayesian models developed. In order to do this, we selected two local SAs: one used in BNs but more commonly in linear modelling (OAT), and one specific for BN modelling (STF).

2.2.1. One-at-a-time

The simplest method to perform a SA is through OAT, in which only one input variable varies at a time while the others remain fixed (Hamby, 1994). Generally, each variable in the model could be changed by a specific amount; for example, all variables were to be increased or decreased by 20% of their original value. For each variable change, the percentage impact on the output variable may be recorded. Through this analysis, it is possible to rank input variables according to their influence on the output variable.

In this case, OAT requires a baseline scenario in which input variables had a uniform probability distribution in order to compare this outcome with outcomes obtained after the analysis. All parameters remained fixed throughout the analysis, while each state of each input variable was varied one at a time alternatively. That is, a particular state reaches a value of 100% leaving the remaining two states at 0. Results for each state of the output variable were compared to the results obtained from the baseline scenario through the following formula:

$$VBS_{i}[\%] = \frac{(Scenario_{new} - Scenario_{baseline})}{Scenario_{baseline}} \times 100$$
(1)

where VBS_i (Variation from the Baseline Scenario) is the relative change in model outcome after changes in the selected input variable (i) (Scenario_{new}) referred to model outcome under the fixed baseline scenario (Scenario_{baseline}).

We obtained a VBS value for each state of input variables over each state of the output variable. In our case, VBS was shown for one state (High) of input variables considering that the response for the other states remain in the same magnitude but to the opposite side. Ecologically, we were only interested in one state of each output variable (i.e. the one directly related to agroecosystems sustainability); that is, High C content in soil, High Available N in soil, Low Denitrification, and Low NO₃ concentration in groundwater (Rositano and Ferraro, 2014) (see Appendix 1). Final results were represented in Tornado diagrams.

2.2.2. Sensitivity to findings

The second SA was done using the STF function from Netica (Chen and Pollino, 2012). STF can use the properties of d-separation (Pollino et al., 2007) which determines whether or not evidence (or findings) about one variable may influence belief in a target variable (Albrecht et al., 2014; Korb and Nicholson, 2004). Through this process, it is

possible to rank input variables according to their influence on the model outcome. Unlike what happens in OAT, an influence value is reported for the whole variable, not for each state. The influence value obtained will change as findings (or evidence) arrive to one or more input variables, so this analysis may need to be recomputed at each stage. Even though it is not considered a problem to do this analysis each time an input variable is quantified, it is possible to obtain a different ranking on each occasion. In BN literature, STF is commonly used after quantifying input variables (e.g. Chen and Pollino, 2012). To avoid this, we decided that input variables would have a uniform probability distribution. We made this assumption because in this way we make results comparable to those obtained with OAT.

The sensitivity of a selected variable could be measured by two indicators: 1) entropy, and 2) mutual information (Pollino et al., 2007). Entropy is the uncertainty ("self-information") of a single random variable, while mutual information is the reduction in uncertainty (i.e. it measures the dependency of two variables). As they are interrelated concepts (i.e. the relationship between both indicators is derived from a mathematical theorem), we decided to focus our analysis on entropy.

Entropy, in ecological terms, is a measure of disorder in a system (Wilkinson, 1963). Considering BNs, entropy (H) is commonly used to evaluate the randomness or uncertainty of a variable characterized by a probability distribution. Its formula is:

$$H(X) = -\sum_{x \notin X} P(x) \log P(x)$$
(2)

where X is a particular variable, and P(x) is the probability distribution which characterizes that variable.

The Shannon (1948) measure of "entropy of information" provides a measure for ranking information sources. It is based on the assumption that the uncertainty regarding any variable X characterized by a probability distribution P(x) can be represented by the entropy function (Grêt-Regamey and Straub, 2006) (Fig. 2). Entropy (H(X)) depends on the probability P(X = 1) that X takes when the value is 1. When P(X = 1) = 0.5, all possible outcomes are equally likely (Fig. 2). Thus, the result is unpredictable and entropy is maximum. For example, a rare event has a lot of information in order to explain the system, while a very common event has little information (Abramson, 1981). In the latter, a situation highly organized (P(x) = 1) is not characterized by a large degree of randomness; that is, the information (or the entropy) is low (H(X) = 0) (Shannon and Weaver, 1964) (Fig. 2).

2.3. Comparison of sensitivity analyses

Both sensitivity techniques have different units in which their outcomes are shown. In order to compare the output of both SAs, we needed to standardize results. Through z-score transformation (Sedgwick, 2014), we could compare them as this method has no units (i.e. numerator and denominator of the ratio are measured in the same units). Its formula is:

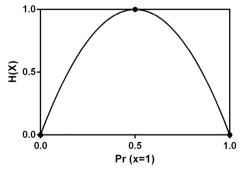


Fig. 2. Entropy (H(X)) curve associated to a range of probabilities.

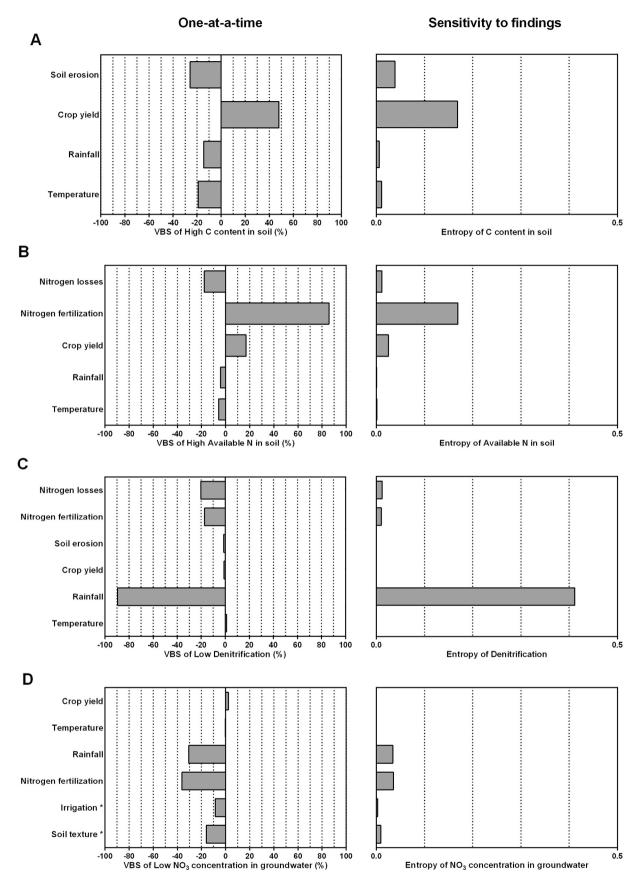


Fig. 3. Sensitivity analyses applied to four Bayesian Networks. Sensitivity analyses were: a) One-at-a-time, and b) Sensitivity to findings. Each pair of graphs (A to D) corresponded to one Bayesian Network. In the case of One-at-a-time, the output variable for each Bayesian Network was: A) High C content in soil, B) High available N in soil, C) Low denitrification, and D) Low NO_3 concentration in groundwater. In the case of Sensitivity to findings, the output variable for each Bayesian Network was: A) C content in soil, B) Available N in soil, C) Denitrification, and D) NO_3 concentration in groundwater. VBS = Variation from the Baseline Scenario; C = Carbono; N = Nitrogen.

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$$z = \frac{x - \mu}{\sigma} \tag{3}$$

where μ is the mean and σ is the standard deviation of the population. This was applied to results obtained from OAT and STF.

3. Results

Both analyses, OAT and STF, produced similar groups of influential variables in our models, although they used completely different computing methods (Fig. 3). Crop yield, Nitrogen fertilization, and Rainfall were the main variables influencing C content in soil, Available N in soil, and Denitrification, respectively (Fig. 3A, B, C). NO $_3$ concentration in groundwater was most influenced by Rainfall and Nitrogen fertilization (Fig. 3D). Rainfall had the least influence over Available N in soil in both SAs (Fig. 3B). Soil erosion, Crop yield, and Temperature had the least influence over Denitrification in both cases (Fig. 3C). Crop yield and Temperature had the least influence over NO $_3$ concentration in groundwater in both SAs (Fig. 3D). Values of input variables which were used to make the ranking are shown in Appendix 2.

OAT detected the direction (positive or negative) of the most influential variables, while STF did not; that is, positive and negative values were obtained during OAT (Fig. 3). Crop yield increased High C content in soil, while Soil erosion decreased it (Fig. 3A). Nitrogen fertilization increased High Available N in soil, and Nitrogen losses decreased it (Fig. 3B). Rainfall increased Low Denitrification, while Temperature decreased it (Fig. 3C). Nitrogen fertilization increased Low NO₃ concentration in groundwater, and Crop yield decreased it (Fig. 3D).

Input variables had similar z-score values between OAT and STF analyses showing that the ordering of these variables by their sensitivity is the same regardless the methodology applied (Fig. 4). In the case of C content in soil, Temperature and Crop yield had a similar z-score value between SAs, while Rainfall and Soil erosion were slightly different (Fig. 4A). In the case of Available N in soil, N losses had different z-score values, while Temperature, Rainfall, Crop yield and Fertilization had similar ones (Fig. 4B). In the case of Denitrification, Rainfall had similar z-score values, while Temperature, Soil erosion, Crop yield, Fertilization and N losses differed in them (Fig. 4C). In the case of NO₃ concentration in groundwater, Soil texture, Irrigation, Rainfall and Temperature had different z-score values, while Fertilization and Crop yield had similar ones (Fig. 4D).

4. Discussion

The main goal of our work was to compare two SAs with different methodological characteristics for assessing BNs in one case study. As was previously introduced, these two analyses measure the effects of individual variable changes; therefore, synergistic effects of changing multiple variables are not detected even though they may be relevant for BNs' predictions (Coupé et al., 1999). Whether global SA techniques could be also employed, such as Latin hypercube sampling method (e.g. Borsuk et al., 2004), two or more variables studied simultaneously could imply difficulties to the interpretation of results (Coupé and van der Gaag, 2002). Based on this, the choice made here (in terms of local SA techniques selected) seems sufficient to provide a general overview of the structural performance of four BNs developed in Rositano and Ferraro (2014). Despite the fact that we obtained the same ranking order of influence of input variables over an output variable, results highlighted the existence of differences and similarities between OAT and STF.

On one hand, a comparison was made according to different aspects of input and output variables. During OAT, we had the opportunity to assess in which way each state of input variables modifies a particular state of the output variable. That is, an input variable increased or diminished the output variable. For example, High Crop yield increased High C content in soil, while High Soil erosion, High Rainfall and High Temperature reduced it (Fig. 3A). The identification of these impacts (positives or negatives) was made possible by Tornado diagrams. A positive impact is shown at the right side of zero, while a negative impact at the left side of zero. This is true only for High C content in soil and High Available N in soil; but in the case of Low Denitrification and Low NO₃ concentration in groundwater, it goes in the opposite direction because we are interested in conserving these externalities in a low degree. During STF, it was not possible to determine if the output variable would increase or diminish through the change on a certain input variable (Fig. 3). STF only informs the ranking of variables, from the most to the least affecting model output. Considering these observed differences, if there is a need to understand the relation (positive or negative) between input and output variables, OAT should be used.

The identification of the most relevant input variables in a model is necessary in order to consider, for example, their usefulness (Bednarski et al., 2004; Confalonieri et al., 2010). Sometimes, such results have led to changes in the network structure. This is the case of input variables with 0 entropy which seem not to play an important role in BNs and, hence, authors have removed them from their models (e.g. Chen and Pollino, 2012). However, an input variable with "no effect, does not mean it does not affect" the output variable (Saltelli and Annoni, 2010). We could check this by applying OAT because it showed that input variables with this characteristic (i.e. 0 entropy in STF) did increase or diminish the output variable in a lesser extent than remaining input variables (Fig. 3). This is the case of Rainfall and Temperature in High Available N in soil (Fig. 3B), Soil erosion, Crop yield and Temperature in Low Denitrification (Fig. 3C), or Crop yield and Temperature in Low NO₃ concentration in groundwater (Fig. 3D). In STF analysis, all these input variables had entropy equal to zero implying that these variables could be excluded from the model. However, they did play a role: increasing or diminishing the model outcome. Here, this could be only discovered with the OAT analysis. Therefore, the need to keep an input variable can arise from applying alternative SA methods. If every sensitivity technique shows that an input variable does not matter, the modeller can decide to take it out from the model (and viceversa).

On the other hand, we obtained the same ranking order of influence of input variables over each output variable in spite of their different magnitudes of change (Fig. 3). This type of result was also obtained by Confalonieri et al. (2010) when applying alternative global SA techniques to the rice model WARM. It is also true that these results could be obtained because of the structure of our models and the range of input values considered. From this ranking, it could be possible to set those input variables in which greater emphasis upon parameterization and quantification should be made (Chen and Pollino, 2012). However, comparing magnitudes of change was not possible because these SAs assessed models with different units. Similarity in z-score values encountered (Fig. 4) set the idea that not only the ranking but also the magnitude are comparable between sensitivity methodologies. Moreover, it could be interesting to understand whether changes in input variables magnify or attenuate the output. Then, if variations in input variables are not proportional or non-linear, uncertainty will propagate through the model reaching the output variable. In relation to this, Bert et al. (2007) proposed a simplified method based on the evaluation of model sensitivity at extreme values of the input variables to evaluate the CERES-Maize model non-linear responses. Considering these observed similarities, OAT and STF could be applied interchangeably, meaning that either one could be used in this case study.

Finally, this comparison was made without populating input variables with realistic quantitative information from a particular study site during STF, which is usually seen in BN literature (e.g. Chen and Pollino, 2012; Grêt-Regamey and Straub, 2006). Populating input variables implies fulfilling them with quantitative information in a probabilistic way. In this case, we did both SAs with no quantitative information (i.e. productive and environmental databases) not because

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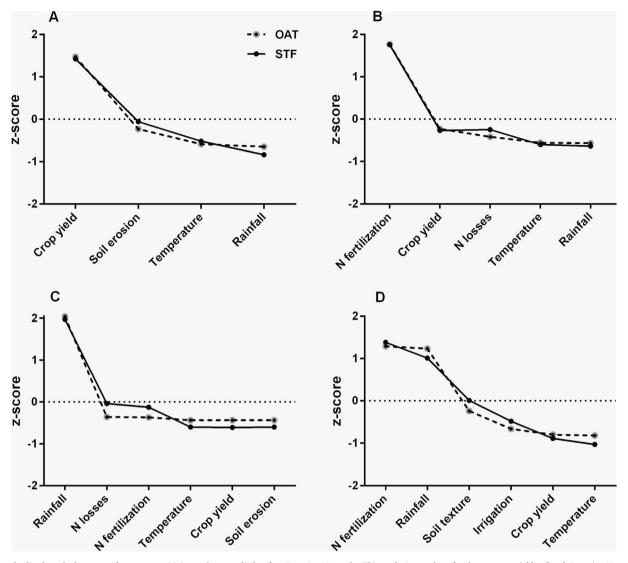


Fig. 4. Standardized results by z-score from two sensitivity analyses applied to four Bayesian Networks. This analysis was done for the output variable of each Bayesian Network: A) C content in soil, B) Available N in soil, C) Denitrification, and D) NO₃ concentration in groundwater. Variables in the X-axes are sorted in view of their influence in the output variable analysed. Dotted lines represent z-score = 0. N = Nitrogen.

of lack of data but because we decided to perform them with a uniform probability distribution in their input variables in order to make both methods comparable. Thus, we do not know if we would have obtained the same ranking of input variables if we had populated them. Our issue highlights the performance of STF in cases where no quantitative information related to a study site is used. Therefore, our future work should be focused on the population of input variables with quantitative information from different study sites in order to assess the ranking of input variables and compare these results with OAT.

5. Conclusions

This paper provided insights about SA methodologies in BNs based on a case study. Specifically, we presented a comparison of two local SAs: one commonly used in linear models (OAT), and another popular within bayesian modellers (STF). We highlighted the existence of differences and similarities between both SAs. All these preliminary identified pros and cons could be of key importance for ecological modellers since SA techniques are an aid in "understanding and manipulating complex models" (Confalonieri et al., 2010), such as OAT and STF for BNs. Even though their interchangeably application could be an alternative in our bayesian models, we believe that OAT is the

suitable one to implement here because of its capacity to demonstrate the relation (positive or negative) between input and output variables.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.ecoinf.2017.07.005.

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